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Generalized bounce back boundary condition for the nine velocities two-dimensional lattice Boltzmann scheme

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Abstract

In a previous work [3], we have proposed a method for the analysis of the bounce back boundary condition with the Taylor expansion method in the linear case. In this work two new schemes of modified bounce back are proposed. The first one is based on the expansion of the iteration of the internal scheme of the lattice Boltzmann method. The analysis puts in evidence some defects and a generalized version is proposed with a set of essentially four possible parameters to adjust. We propose to reduce this number to two with the elimination of spurious density first order terms. Thus a new scheme for bounce back is found exact up to second order and allows an accurate simulation of the Poiseuille flow for a specific combination of the relaxation and boundary coefficients. We have validated the general expansion of the value in the first cell in terms of given values on the boundary for a stationary “accordion” test case.

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Introduction

In this contribution, we study boundary conditions for lattice Boltzmann schemes using the Taylor expansion method proposed in our previous work [3]. In that work, we have proposed a method for the analysis of the bounce back boundary condition in the particular case of the D2Q9 scheme [7] for a bottom boundary. Note that the bounce back boundary condition and anti-bounce back boundary condition were studied by Ginzburg and Adler [5], Zou and He [8], Bouzidi *et al* [1] and d’Humières and Ginzburg [6]. A particular choice of the LB parameters can enhance the precision of the scheme.

In this contribution, more general bounce back boundary conditions are proposed. We follow the same method as in [3] to analyze the proposed scheme up to second order in space. Three schemes are investigated and implemented for a Poiseuille flow with an imposed pressure field at the input and at the output of the domain. Finally, we propose a new scheme for bounce back exact up to order two in space that allows an accurate simulation of the Poiseuille flow for any combination of the relaxation coefficients.

1) D2Q9 lattice Boltzmann scheme

The D2Q9 lattice Boltzmann schemes uses a set of discrete velocities described in Fig. 1. A density distribution f_j is associated to each velocity $v_j \equiv \lambda e_j$, where $\lambda = \frac{\Delta x}{\Delta t}$ is the fixed numerical lattice velocity. From this particle distribution, we construct a vector m of moments m_k according to

$$(1) \quad m = M f$$

with an inversible fixed matrix M usually [7] given by

$$(2) \quad M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{pmatrix}.$$

The three first moments for the density and momentum are defined according to

$$(3) \quad \rho = \sum_{j=0}^8 f_j = m_0, \quad j_x \equiv \rho u_x = \sum_{j=0}^8 \lambda e_j^1 f_j = m_1, \quad j_y \equiv \rho u_y = \sum_{j=0}^8 \lambda e_j^2 f_j = m_2,$$

where e_j^α are the cartesian components of the vectors e_j introduced previously. For fluid mechanics applications, a set of “conserved variables” W is defined by

$$(4) \quad W = (\rho, j_x, j_y).$$

The moment distribution at equilibrium m^{eq} is a function of the conserved variables only. In particular, the equilibrium value of the fourth moment associated to kinetic energy (see the fourth line in the matrix M presented in (2)) is parametrized with the help of a constant α .

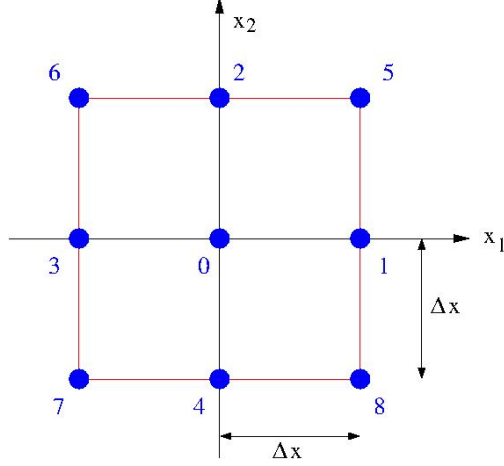


Figure 1: Particle distribution f_j for $0 \leq j \leq 8$ of the D2Q9 lattice Boltzmann scheme.

For the equilibrium of the last moment (of fourth order), we introduce a constant β , as in our previous work [3]. Note that the standard D2Q9 scheme [7] uses $\alpha = -2$ and $\beta = 1$. The vector m^{eq} of equilibrium moments is defined according to:

$$(5) \quad m^{\text{eq}} = (\rho, j_x, j_y, \alpha \lambda^2 \rho, 0, 0, -\lambda^2 j_x, -\lambda^2 j_y, \beta \lambda^4 \rho)^{\text{t}}.$$

Applying the inverse of relation (1) with the matrix M defined in (2), we can explicit herein all the components of the vector f^{eq} :

$$(6) \quad f^{\text{eq}} : \begin{cases} f_0^{\text{eq}} = \frac{\rho}{9} [1 - \alpha + \beta], \\ f_1^{\text{eq}} = \frac{\rho}{36} \left[4 - \alpha - 2\beta + \frac{12 u_x}{\lambda} \right], \\ f_2^{\text{eq}} = \frac{\rho}{36} \left[4 - \alpha - 2\beta + \frac{12 u_y}{\lambda} \right], \\ f_3^{\text{eq}} = \frac{\rho}{36} \left[4 - \alpha - 2\beta - \frac{12 u_x}{\lambda} \right], \\ f_4^{\text{eq}} = \frac{\rho}{36} \left[4 - \alpha - 2\beta - \frac{12 u_y}{\lambda} \right], \\ f_5^{\text{eq}} = \frac{\rho}{36} \left[4 + 2\alpha + \beta + \frac{3}{\lambda} (u_x + u_y) \right], \\ f_6^{\text{eq}} = \frac{\rho}{36} \left[4 + 2\alpha + \beta + \frac{3}{\lambda} (-u_x + u_y) \right], \\ f_7^{\text{eq}} = \frac{\rho}{36} \left[4 + 2\alpha + \beta + \frac{3}{\lambda} (-u_x - u_y) \right], \\ f_8^{\text{eq}} = \frac{\rho}{36} \left[4 + 2\alpha + \beta + \frac{3}{\lambda} (u_x - u_y) \right]. \end{cases}$$

The lattice Boltzmann scheme is composed of two fundamental steps : relaxation and advection. During the relaxation step, the conserved variables $W \equiv (\rho, J_x, J_y)$ are not modified; the nonconserved moments m_3 to m_8 relax towards an equilibrium value :

$$m_k^{\text{eq}} = \psi_k(W) \quad \text{for } k \geq 3,$$

where the ψ_k are linear functions of the conserved moments given in (5). This step depends upon relaxation rates s_k for $k \geq 3$:

$$m_k^* = m_k + s_k (m_k^{\text{eq}} - m_k),$$

where superscript $*$ denotes the moment m_k after relaxation step. Now using the matrix M^{-1} the relaxation step becomes in the f space :

$$(7) \quad f_i^*(x, t) = \sum_{\ell} M_{i\ell}^{-1} m_{\ell}^*.$$

During the advection step $f_i(x_j)$ is “transported” from the node x_j according to the discrete velocity v_i to the node $x_j + v_i \Delta t$. Thus the evolution of populations f_i $0 \leq i \leq 8$, at internal node x is described by :

$$(8) \quad f_i(x, t + \Delta t) = f_i^*(x - v_i \Delta t, t).$$

2) Bounce back boundary conditions for the D2Q9 scheme

Let us consider, without loss of generality, the bottom boundary configuration as described in Fig. 2. The values $f_i^*(x - v_i \Delta t)$ for $i \in \{2, 5, 6\} \equiv \mathcal{B}$ to perform the scheme are unknown.

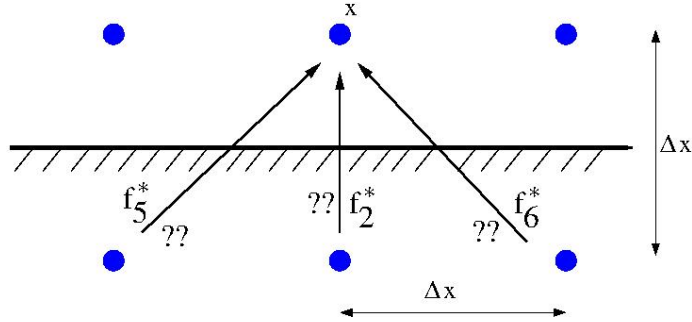


Figure 2: Missing distribution functions to define the boundary scheme for the D2Q9 on a boundary located at $y = 0$.

To impose a given velocity (J_x, J_y) on the boundary we apply bounce back boundary condition :

$$(9) \quad \begin{cases} f_2(x, t + \Delta t) = f_4^*(x) + \frac{2}{3\lambda} J_y \left(x, t + \frac{\Delta t}{2} \right), \\ f_5(x, t + \Delta t) = f_7^*(x) + \frac{1}{6\lambda} (J_x + J_y) \left(x - \frac{\Delta x}{2}, t + \frac{\Delta t}{2} \right), \\ f_6(x, t + \Delta t) = f_8^*(x) + \frac{1}{6\lambda} (-J_x + J_y) \left(x + \frac{\Delta x}{2}, t + \frac{\Delta t}{2} \right). \end{cases}$$

The bounce back scheme (9) can be explained by a very simple idea : apply the internal scheme at the boundary. If we focus on f_2 , we have $f_2(x, t + \Delta t) = f_2^*(x - (0, \Delta x), t)$. For an internal node x the particle distribution f_j is close to the equilibrium idem for the particle distribution f_j^* after collision. So a simple calculus leads to :

$$f_2^*(x - (0, \Delta x)) - f_4^*(x) = f_2^{\text{eq}}(x) - f_4^{\text{eq}}(x) + O(\Delta x).$$

Now we replace f^{eq} by their values given by (6), we get

$$\begin{aligned} f_2^*(x - (0, \Delta x)) - f_4^*(x) &= \frac{\rho}{36} \left[4 - \alpha - 2\beta + \frac{12u_y}{\lambda} \right] - \frac{\rho}{36} \left[4 - \alpha - 2\beta - \frac{12u_y}{\lambda} \right] + O(\Delta x) \\ &= \frac{2}{3\lambda} J_y(x) + O(\Delta x). \end{aligned}$$

We remark here that ρu_y was substituted by the given function J_y on the boundary which is the non-homogenous velocity to impose. An analogous calculus for the two other expressions gives the scheme (9).

- When the boundary condition is taken in a nonlinear way, the particle distribution at equilibrium is taken as a nonlinear function of the conserved quantities. Then taking appropriate sums and differences of the corresponding relations that generalize (6), the extension of the bounce back conditions (9) to the nonlinear framework is elementary. Our present analysis method is completely linear and we do not consider the nonlinear framework in this contribution.

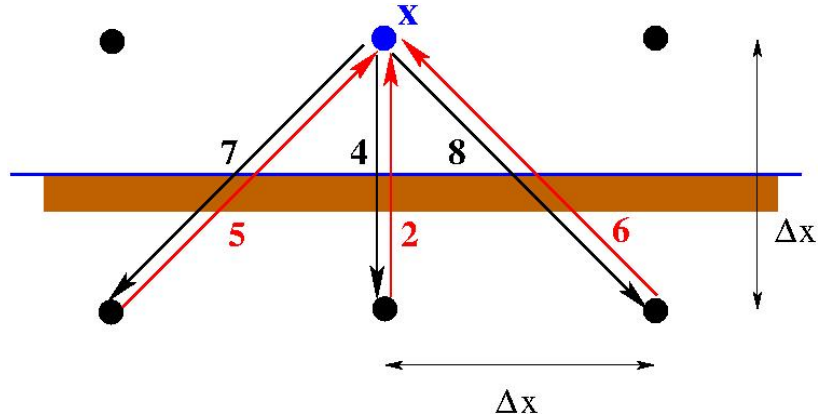


Figure 3: Bounce back scheme for bottom boundary configuration with the D2Q9 scheme.

- **Analysis of bounce back boundary condition.**

In a previous work [3] we made an analysis of the bounce back scheme using Taylor development which provides a development of the velocity on the boundary node up to order two in space.

The main result is the following proposition.

Proposition 1.

Expansion of momentum at the node near the boundary up to order two

The momentum (J_x, J_y) (with upper-case letters) is given on the boundary (see Figure 4). In this proposition, we expand the momentum (j_x, j_y) (with lower-case letters) at the vertex

x , located half a mesh size over the boundary, in terms of these data. We have

$$(10) \quad \left\{ \begin{array}{l} j_x = J_x - \frac{\Delta t}{2} (4\sigma_7 + 3) \partial_t J_x + \frac{\Delta x}{2} \partial_y J_x \\ \quad + \lambda \Delta x \left(\frac{3\alpha + 2\beta + 4}{6} \sigma_7 - \frac{\alpha + 4}{6} \left(2\sigma_7 + \frac{3}{2} \right) \right) \partial_x \rho \\ \quad + \Delta x^2 \left[\alpha_{tt}^0 \partial_t^2 J_x + \alpha_{ty}^0 \partial_t \partial_y J_x + \alpha_{xx}^0 \partial_x^2 J_x + \alpha_{yy}^0 \partial_y^2 J_x + \beta_{tx}^0 \partial_t \partial_x J_y, \right. \\ \quad \left. + \beta_{xy}^0 \partial_{xy}^2 J_y + \gamma_{ty}^0 \partial_{tx}^2 J_y + \gamma_{xy}^0 \partial_x \partial_y \rho \right] + O(\Delta x^3) \\ j_y = J_y - \frac{\Delta t}{2} \partial_t J_y + \frac{\Delta x}{2} \partial_y J_y - \frac{\Delta x}{12} (\alpha + 4) \partial_y \rho \\ \quad + \Delta x^2 \left[\theta_{tx}^0 \partial_t \partial_x J_x + \theta_{xy}^0 \partial_x \partial_y J_x + \eta_{tt}^0 \partial_t^2 J_y + \eta_{ty}^0 \partial_t \partial_y J_y + \eta_{xx}^0 \partial_x^2 J_y \right. \\ \quad \left. + \eta_{yy}^0 \partial_y^2 J_y + \zeta_{ty}^0 \partial_t \partial_y \rho + \zeta_{yy}^0 \partial_y^2 \rho \right] + O(\Delta x^3). \end{array} \right.$$

The coefficients that parametrize the second order terms in (10) can be explicitly evaluated and we have

$$(11) \quad \left\{ \begin{array}{l} \alpha_{tt}^0 = \frac{1}{\lambda^2} \left(6\sigma_7^2 + 6\sigma_7 + \frac{13}{8} \right), \quad \alpha_{ty}^0 = -\frac{1}{2\lambda} (2\sigma_7 + 3\sigma_4 + 3), \\ \alpha_{xx}^0 = \frac{1}{24} (24\sigma_4\sigma_7 + 8\sigma_7\sigma_8 + 12\sigma_4 + 8\sigma_7 + 15), \quad \alpha_{yy}^0 = \frac{1}{4} (2\sigma_4 + 1), \\ \beta_{tx}^0 = \frac{1}{12\lambda} (12\sigma_4\sigma_7 - 4\sigma_7\sigma_8 + 6\sigma_4 - 4\sigma_7 - 9), \\ \beta_{xy}^0 = -\frac{1}{12} (12\sigma_4\sigma_7 - 4\sigma_7\sigma_8 - 4\sigma_7 - 9), \\ \gamma_{tx}^0 = -\frac{1}{12} (2\alpha\sigma_3\sigma_7 + 6\alpha\sigma_7^2 + 12\beta\sigma_7^2 + 4\beta\sigma_7\sigma_8 - 3\alpha\sigma_3 - 3\alpha\sigma_7 \\ \quad + 6\beta\sigma_7 - 24\sigma_7^2 - 5\alpha - \beta - 40\sigma_7 - 22), \\ \gamma_{xy}^0 = \frac{\lambda}{36(2\sigma_7 + 1)} (6\alpha\sigma_3\sigma_7^2 - 6\alpha\sigma_4\sigma_7^2 + 8\alpha\sigma_7^2\sigma_8 + 4\beta\sigma_3\sigma_7^2 - 12\beta\sigma_4\sigma_7^2 \\ \quad + 8\beta\sigma_7^2\sigma_8 - 9\alpha\sigma_3\sigma_7 - 15\alpha\sigma_4\sigma_7 - 4\alpha\sigma_7^2 - 2\alpha\sigma_7\sigma_8 \\ \quad - 6\beta\sigma_3\sigma_7 - 6\beta\sigma_4\sigma_7 + 8\sigma_3\sigma_7^2 + 24\sigma_4\sigma_7^2 - 6\alpha\sigma_4 \\ \quad - 29\alpha\sigma_7 - 6\beta\sigma_7 - 12\sigma_3\sigma_7 - 36\sigma_4\sigma_7 - 16\sigma_7^2 - 8\sigma_7\sigma_8 - 9\alpha \\ \quad - 24\sigma_4 - 92\sigma_7 - 36), \\ \theta_{tx}^0 = -\frac{1}{4\lambda} (2\sigma_4 + 1), \quad \theta_{xy}^0 = \frac{1}{4}, \quad \eta_{tt}^0 = \frac{1}{8\lambda^2}, \quad \eta_{ty}^0 = -\frac{1}{6\lambda} (\sigma_4 + 4), \quad \eta_{xx}^0 = \frac{4\sigma_4 + 1}{24}, \\ \eta_{yy}^0 = \frac{1}{12} (2\sigma_4 + 5), \quad \zeta_{ty}^0 = \frac{1}{24} (2\alpha\sigma_3 + \alpha + 8), \quad \zeta_{xx}^0 = -\frac{\lambda}{24} (2\sigma_4 + 1)(\alpha + 4), \\ \zeta_{yy}^0 = -\frac{\lambda}{72(1 + 2\sigma_7)} (6\alpha\sigma_3\sigma_7 - 2\alpha\sigma_4\sigma_7 + 4\beta\sigma_3\sigma_7 - 4\beta\sigma_4\sigma_7 + 2\alpha\sigma_4 \\ \quad + 10\alpha\sigma_7 + 8\sigma_3\sigma_7 + 8\sigma_4\sigma_7 + 5\alpha + 8\sigma_4 + 40\sigma_7 + 20). \end{array} \right.$$

Remark

We summarize here the demonstration established in our previous work [3] to use its results later and make this paper independent and clear.

Proof of Proposition 1.

We write bounce back in general form :

$$(12) \quad f_j^*(x, t + \Delta t) = f_\ell^*(x, t) + \xi_j(x', t'), \quad j \in \mathcal{B},$$

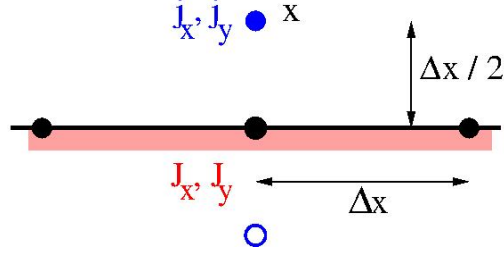


Figure 4: Expansion of the momentum (j_x, j_y) in the first cell as a function of the data (J_x, J_y) on the boundary.

where ℓ is opposite of j (*i.e.* $v_j + v_\ell = 0$) and $\xi_j(x', t')$ is the given velocity on the boundary as *e.g.* proposed in (9) to fix the ideas. If $j \notin \mathcal{B}$ the above equation is replaced by the internal scheme (8). By introducing tables $T_{j,\ell}$, and $U_{j,\ell}$ the unified expression of the lattice Boltzmann scheme for a node x near the boundary is given by

$$(13) \quad f_j(x, t + \Delta t) = \sum_{\ell} T_{j,\ell} f_{\ell}^*(x, t) + \sum_{\ell} U_{j,\ell} f_{\ell}^*(x - v_j \Delta t, t) + \xi_j$$

where the matrix $U_{j,\ell} = 1$ if $\ell = j \notin \mathcal{B}$ and $U_{j,\ell} = 0$ if not. The matrix U describes the “internal” numerical scheme (8) whereas the matrix T takes into account the bounce back boundary scheme (9). For the particular bottom boundary with the D2Q9 scheme as presented in Fig. 3, the tables U and T are :

$$(14) \quad U = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

After linearization of the equilibrium, we can write the relaxation step as follows :

$$m^* = J_0 m,$$

with

$$(15) \quad J_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha s_3 \lambda^2 & 0 & 0 & 1 - s_3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 - s_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 - s_4 & 0 & 0 & 0 \\ 0 & -s_7 \lambda^2 & 0 & 0 & 0 & 0 & 1 - s_7 & 0 & 0 \\ 0 & 0 & -s_7 \lambda^2 & 0 & 0 & 0 & 0 & 1 - s_7 & 0 \\ \beta s_8 \lambda^4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 - s_8 \end{pmatrix}.$$

Then the unified LB scheme (13) for the bounce back becomes :

$$(16) \quad \begin{cases} m_k(x, t + \Delta t) = (MTM^{-1}J_0)_{k,\ell} m_\ell(x, t) \\ \quad \quad \quad + (M_{k,\ell}U_{\ell,j}M_{j,p}^{-1}(J_0)_{p,q}) m_q(x - v_\ell\Delta t, t) + M_{k,\ell} \xi_\ell, \end{cases}$$

with an implicit summation on the repeated indices. We expand this relation to order 0, 1 and 2.

- Analysis of bounce back at order zero

Let us introduce the matrix $K \equiv I - M(T + U)M^{-1}J_0$, where I is the identity matrix. Then the equivalent equations for bounce back scheme at order zero are the solution of

$$(17) \quad Km = M\xi + O(\Delta x).$$

For the D2Q9 scheme the matrix K is given by :

$$(18) \quad K = \begin{pmatrix} 0 & 0 & \frac{1}{\lambda} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{2-s_7}{3} & 0 & 0 & 0 & 0 & \frac{1-s_7}{3\lambda^2} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -s_3\alpha\lambda^2 & 0 & \lambda(1-s_7) & s_3 & 0 & 0 & 0 & \frac{1-s_7}{\lambda} & 0 \\ 0 & 0 & -\frac{\lambda(1+s_7)}{3} & 0 & s_4 & 0 & 0 & \frac{1-s_7}{3\lambda} & 0 \\ 0 & \frac{\lambda(2-s_7)}{3} & 0 & 0 & 0 & s_4 & \frac{1-s_7}{3\lambda} & 0 & 0 \\ 0 & \frac{2\lambda^2(1+s_7)}{3} & 0 & 0 & 0 & 0 & \frac{1+2s_7}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -\beta s_8\lambda^4 & 0 & -s_7\lambda^3 & 0 & 0 & 0 & 0 & \lambda(1-s_7) & s_8 \end{pmatrix}.$$

We remark that the matrix K is singular and the dimension of its kernel is equal to 1. In fact with $\mu_0 \equiv (1, 0, 0, \alpha\lambda^2, 0, 0, 0, 0, \beta\lambda^4)^t$, we have $K\mu_0 = 0$.

In consequence, we have one compatibility relation to satisfy, it is a linear combination of the equivalent equations of the internal scheme :

$$\lambda(\partial_t\rho + \partial_x j_x + \partial_y j_y) - \left(\partial_t j_y + \frac{\alpha+4}{6}\lambda^2\partial_y\rho\right) = O(\Delta x).$$

With given momenta J_x and J_y on the boundary, the density ρ remains still undefined by the boundary scheme. We develop the moments m as : $m = m_0 + \Delta t m_1 + O(\Delta t^2)$. We find that the solution of (17) at order zero is :

$$m_0 = (\rho, J_x, J_y, \alpha\rho\lambda^2, 0, 0, -\lambda^2 J_x, -\lambda^2 J_y, \beta\rho\lambda^4)^t.$$

- Analysis of bounce back at order one

Let introduce the matrix

$$B_{k,p}^\alpha = \sum_{\ell,j,q} M_{k,\ell} U_{\ell,j} v_j^\alpha M_{j,q}^{-1} (J_0)_{q,p}, \quad \alpha = 1, 2.$$

Then the equivalent equations for bounce back scheme up to order one are solutions of

$$Km = M\xi + \Delta t [M\partial\xi - \partial_t m - B^\alpha\partial_\alpha m] + O(\Delta x^2),$$

with $m = m_0 + \Delta t m_1 + O(\Delta x^2)$, and we have

$$m_1 = \Sigma \cdot (M\partial\xi - \partial_t m_0 - B^\alpha\partial_\alpha m_0).$$

The matrix Σ is given by :

$$(19) \quad \Sigma = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 + \frac{1}{s_7} & 0 & 0 & 0 & 0 & \frac{1}{\lambda^2} \left(1 - \frac{1}{s_7}\right) & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\lambda}{s_3} (s_7 - 1) & \frac{1}{s_3} & 0 & 0 & 0 & \frac{1}{\lambda s_3} (s_7 - 1) & 0 \\ 0 & 0 & \frac{\lambda}{3 s_4} (1 + s_7) & 0 & \frac{1}{s_4} & 0 & 0 & \frac{s_7 - 1}{3 \lambda s_4} & 0 \\ 0 & -\frac{\lambda}{s_4} & 0 & 0 & 0 & \frac{1}{s_4} & 0 & 0 & 0 \\ 0 & -2\lambda^2 \left(1 + \frac{1}{s_7}\right) & 0 & 0 & 0 & 0 & \frac{2}{s_7} - 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \lambda^3 \frac{s_7}{s_8} & 0 & 0 & 0 & 0 & \frac{\lambda}{s_8} (s_7 - 1) & \frac{1}{s_8} \end{pmatrix}.$$

- Analysis of bounce back at order two

Let us introduce the matrix $\tilde{B}_{k,\ell}^{\alpha,\beta} = \sum_{k,j,p,q} M_{k,p} U_{p,j} v_j^\alpha v_j^\beta M_{j,q}^{-1} (J_0)_{q,\ell}$, $1 \leq \alpha, \beta \leq 2$.

Then expand the various terms of the relation (16) up to second order. We get the following equation :

$$(20) \quad \begin{cases} Km = M\xi + \Delta t [M\partial\xi - \partial_t m - B^\alpha \partial_\alpha m] \\ + \frac{1}{2} \Delta t^2 [M\partial^2 \xi - \partial_t^2 m \tilde{B}^{\alpha,\beta} \partial_\alpha \partial_\beta m] + O(\Delta t^3). \end{cases}$$

Now we develop m as : $m = m_0 + \Delta t m_1 + \Delta t^2 m_2 + O(\Delta x^3)$. We get m_2 as solution of the equation (20) :

$$m_2 = K^{-1} \cdot \left[-\partial_t m_1 - B^\alpha \partial_\alpha m_1 + \frac{1}{2} \left(M\partial^2 \xi - \partial_t^2 m_0 + \tilde{B}^{\alpha,\beta} \partial_\alpha \partial_\beta m_0 \right) \right].$$

Finally the development of the velocities on the boundary nodes are given by the second and third components of $m = m_0 + \Delta t m_1 + \Delta t^2 m_2 + O(\Delta x^3)$. When we explicit the conserved moments, the previous relation leads to the relation (10). \square

- We can use the equivalent partial differential equations of the internal scheme derived with the initial Taylor expansion method in order to express the relations (10) and (11) without the time derivatives. Recall that we have in the linearized case

$$(21) \quad \begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = O(\Delta x^2), \\ \partial_t j_x + c_0^2 \partial_x \rho - \frac{\lambda^2 \Delta t}{3} \sigma_4 (\partial_x^2 + \partial_y^2) j_x + \frac{\lambda^2 \Delta t}{6} \sigma_3 \alpha \partial_x (\partial_x j_x + \partial_y j_y) = O(\Delta x^2), \\ \partial_t j_y + c_0^2 \partial_y \rho - \frac{\lambda^2 \Delta t}{3} \sigma_4 (\partial_x^2 + \partial_y^2) j_y + \frac{\lambda^2 \Delta t}{6} \sigma_3 \alpha \partial_y (\partial_x j_x + \partial_y j_y) = O(\Delta x^2), \end{cases}$$

where $c_0 = \lambda \sqrt{\frac{\alpha + 4}{6}}$ is the speed of sound.

In the result proposed in Proposition 1, we can take into account time dependent velocity data on the boundary. In the following proposition, we transform the first and second order time derivatives introduced in the expansion (10) with the help of the partial differential equations presented at the relations (21). We obtain after a tedious computation a new

expression of the momentum in the cell directly close to the boundary.

Proposition 2.

A second expression of the velocity up to order two at the boundary node

We have the following expansions of the values j_x, j_y at the boundary node in terms of the exact solution J_x, J_y on the boundary (at $x - \frac{\Delta x}{2}$):

$$(22) \quad \left\{ \begin{array}{l} j_x = J_x + \frac{\Delta x}{2} \partial_y J_x + \frac{\lambda \Delta x}{6} (3\alpha + 2\beta + 4) \sigma_7 \partial_x \rho \\ \quad + \Delta x^2 \left[\tilde{\alpha}_{xx}^0 \partial_x^2 J_x + \tilde{\alpha}_{yy}^0 \partial_y^2 J_x + \tilde{\beta}_{xy}^0 \partial_{xy}^2 J_y + \tilde{\gamma}_{xy}^0 \partial_x \partial_y \rho \right] + O(\Delta x^3), \\ j_y = J_y + \frac{\Delta x}{2} \partial_y J_y - \frac{\Delta x}{12} (\alpha + 4) \partial_y \rho \\ \quad + \Delta x^2 \left[\tilde{\theta}_{xy}^0 \partial_x \partial_y J_x + \tilde{\eta}_{xx}^0 \partial_x^2 J_y + \tilde{\eta}_{yy}^0 \partial_y^2 J_x + \tilde{\zeta}_{yy}^0 \partial_y^2 \rho \right] + O(\Delta x^3), \end{array} \right.$$

with

$$(23) \quad \left\{ \begin{array}{l} \tilde{\alpha}_{xx}^0 = \frac{1}{48} (24\alpha\sigma_3\sigma_7 + 72\alpha\sigma_7^2 + 48\beta\sigma_7^2 + 16\beta\sigma_7\sigma_8 + 36\alpha\sigma_7 + 24\beta\sigma_7 \\ \quad + 16\sigma_4\sigma_7 + 96\sigma_7^2 + 16\sigma_7\sigma_8 - 7\alpha - 4\beta + 48\sigma_7 - 6), \\ \tilde{\alpha}_{yy}^0 = -\frac{1}{12} (8\sigma_4\sigma_7 - 3), \\ \tilde{\beta}_{xy}^0 = \frac{1}{48} (24\alpha\sigma_3\sigma_7 + 72\alpha\sigma_7^2 + 48\beta\sigma_7^2 + 16\beta\sigma_7\sigma_8 + 36\alpha\sigma_7 + 24\beta\sigma_7 - 48\sigma_4\sigma_7 \\ \quad + 96\sigma_7^2 + 16\sigma_7\sigma_8 - 7\alpha - 4\beta + 48\sigma_7), \\ \tilde{\gamma}_{xy}^0 = \frac{\lambda}{72(2\sigma_7 + 1)} (12\alpha\sigma_3\sigma_7^2 - 36\alpha\sigma_4\sigma_7^2 + 24\alpha\sigma_7^2\sigma_8 + 8\beta\sigma_3\sigma_7^2 - 24\beta\sigma_4\sigma_7^2 \\ \quad + 16\beta\sigma_7^2\sigma_8 - 18\alpha\sigma_3\sigma_7 - 18\alpha\sigma_4\sigma_7 + 24\alpha\sigma_7^2 - 12\beta\sigma_3\sigma_7 \\ \quad - 12\beta\sigma_4\sigma_7 + 16\sigma_3\sigma_7^2 - 48\sigma_4\sigma_7^2 + 32\sigma_7^2\sigma_8 + 12\alpha\sigma_7 - 12\beta\sigma_7 \\ \quad - 24\sigma_3\sigma_7 - 24\sigma_4\sigma_7 + 96\sigma_7^2 + 9\alpha + 96\sigma_7 + 36), \\ \tilde{\theta}_{xy}^0 = -\frac{\alpha}{48}, \tilde{\eta}_{xx}^0 = \frac{1}{24}, \tilde{\eta}_{yy}^0 = -\frac{1}{48} (\alpha - 8), \\ \tilde{\zeta}_{yy}^0 = -\frac{\lambda}{72(1 + 2\sigma_7)} (6\alpha\sigma_3\sigma_7 - 6\alpha\sigma_4\sigma_7 + 4\beta\sigma_3\sigma_7 - 4\beta\sigma_4\sigma_7 - 6\alpha\sigma_7 \\ \quad + 8\sigma_3\sigma_7 - 8\sigma_4\sigma_7 - 3\alpha - 24\sigma_7 - 12). \end{array} \right.$$

Remark

We have validated all the stationary coefficients of the equation (10) by different numerical test cases [3].

3) Towards a generalized first order bounce back boundary condition

To get a generalized first order bounce back scheme the idea is to apply the internal scheme at the boundary

$$(24) \quad \left\{ \begin{array}{l} f_5(x, t + \Delta t) = f_5^*(x - (\Delta x, \Delta x), t), \\ f_2(x, t + \Delta t) = f_2^*(x - (0, \Delta x), t), \\ f_6(x, t + \Delta t) = f_6^*(x + (\Delta x, -\Delta x), t). \end{array} \right.$$

Then the expressions :

$$(25) \quad \begin{cases} b_l & \equiv f_5^*(x - (\Delta x, \Delta x)) - f_7^*(x), \\ b_m & \equiv f_2^*(x - (0, \Delta x)) - f_4^*(x), \\ b_r & \equiv f_6^*(x + (\Delta x, -\Delta x), t) - f_8^*(x), \end{cases}$$

are expanded at order one.

Remark

If the expressions b_l , b_m and b_r are expanded only to order zero we get the traditional bounce back.

Proposition 3. First order bounce back

For the boundary configuration described in Fig. 3, the bounce back of first order scheme is given as follows :

$$(26) \quad \begin{cases} f_5(x, t + \Delta t) = f_7^*(x) + \frac{1}{6\lambda} (J_x + J_y) \left(x - \frac{\Delta x}{2}\right) + \frac{1}{6} (q_x^* + q_y^* + \frac{1}{\lambda} (j_x + j_y)) \\ \quad \quad \quad + \frac{4 + \beta + 2\alpha}{36} (\rho(x) - \rho(x + (\Delta x, \Delta x))), \\ f_2(x, t + \Delta t) = f_4^*(x) + \frac{2}{3\lambda} J_y(x) - \frac{1}{3} (q_y^*(x) + \frac{1}{\lambda} j_y(x)) \\ \quad \quad \quad + \frac{4 - 2\beta - \alpha}{36} (\rho(x) - \rho(x + (0, \Delta x))), \\ f_6(x, t + \Delta t) = f_8^*(x) - \frac{1}{6\lambda} (J_x - J_y) \left(x + \frac{\Delta x}{2}\right) + \frac{1}{6} (-q_x^* + q_y^* + \frac{1}{\lambda} (-j_x + j_y)) \\ \quad \quad \quad + \frac{4 + \beta + 2\alpha}{36} (\rho(x) - \rho(x + (-\Delta x, \Delta x))). \end{cases}$$

Proof of Proposition 3.

We use Taylor expansion for the expressions b_l , b_m and b_r (see equations 25), we get :

$$(27) \quad \begin{cases} b_l & = f_5^*(x) - f_7^*(x) + df_5^{\text{eq}}(x) \bullet (-\Delta x, -\Delta x) + O(\Delta x^2), \\ b_m & = f_2^*(x) - f_4^*(x) + df_2^{\text{eq}}(x) \bullet (0, -\Delta x) + O(\Delta x^2), \\ b_r & = f_6^*(x) - f_8^*(x) + df_6^{\text{eq}}(x) \bullet (\Delta x, -\Delta x) + O(\Delta x^2). \end{cases}$$

With the help of (7), we obtain the following exact expressions :

$$(28) \quad \begin{cases} f_5^* - f_7^* & \equiv \frac{1}{3\lambda} (j_x + j_y) + \frac{1}{6} (q_x^* + q_y^*), \\ f_2^* - f_4^* & \equiv \frac{1}{3\lambda} j_y - \frac{1}{3} q_y^*, \\ f_6^* - f_8^* & \equiv -\frac{1}{3\lambda} (j_x - j_y) - \frac{1}{6} (q_x^* - q_y^*). \end{cases}$$

On the other hand, we use the expressions (6) for f_j^{eq} , for j equals 2, 5 and 6. So we have for D2Q9 particle equilibrium distribution :

$$(29) \quad \begin{cases} f_5^{\text{eq}} & = \frac{1}{36} (4 + 2\alpha + \beta) \rho + \frac{1}{12\lambda} (j_x + j_y), \\ f_2^{\text{eq}} & = \frac{1}{36} (4 - \alpha - 2\beta) \rho + \frac{1}{3\lambda} j_y, \\ f_6^{\text{eq}} & = \frac{1}{36} (4 + 2\alpha + \beta) \rho - \frac{1}{12\lambda} (j_x - j_y). \end{cases}$$

In the expression (27) we need to expand df_j^{eq} for j equals 2, 5 and 6. Taking into account the above equations we need to develop the gradient of density and the gradient of momentum.

- Gradient of density : using a Taylor expansion of the density around the node x (see Fig. 5) we get :

$$(30) \quad \begin{cases} \nabla \rho \cdot (\Delta x, \Delta x) \simeq \rho(x + (\Delta x, \Delta x)) - \rho(x) + O(\Delta x^2), \\ \nabla \rho \cdot (0, \Delta x) \simeq \rho(x + (0, \Delta x)) - \rho(x) + O(\Delta x^2), \\ \nabla \rho \cdot (-\Delta x, \Delta x) \simeq \rho(x + (-\Delta x, \Delta x)) - \rho(x) + O(\Delta x^2). \end{cases}$$

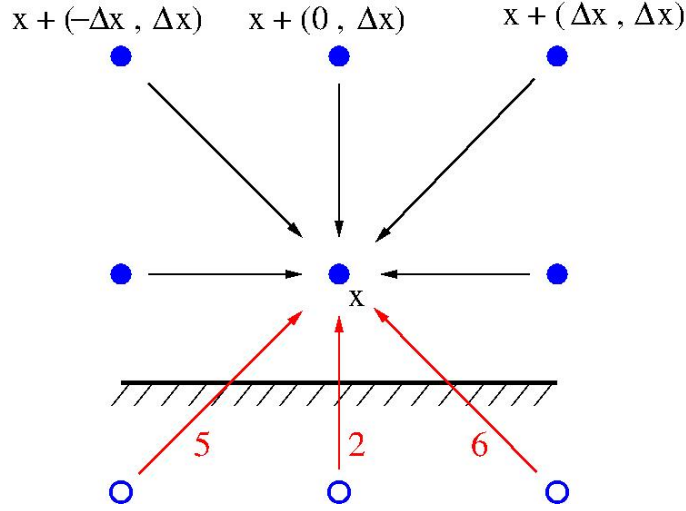


Figure 5: Node near the boundary for the D2Q9 scheme.

- Gradient of momentum : using again Taylor expansion of the following combinations of the momentum around the node x (see Fig. 6) we get :

$$(31) \quad \begin{cases} \nabla(j_x + j_y) \cdot (\Delta x, \Delta x) \simeq 2 \left[(j_x(x) + j_y(x)) - (J_x + J_y) \left(x - \frac{\Delta x}{2} \right) \right] + O(\Delta x^2), \\ \nabla j_y \cdot (0, \Delta x) \simeq 2 (j_y(x) - J_y(x)) + O(\Delta x^2), \\ \nabla(j_x - j_y) \cdot (-\Delta x, \Delta x) \simeq 2 \left[(j_x(x) - j_y(x)) - (J_x - J_y) \left(x + \frac{\Delta x}{2} \right) \right] + O(\Delta x^2). \end{cases}$$

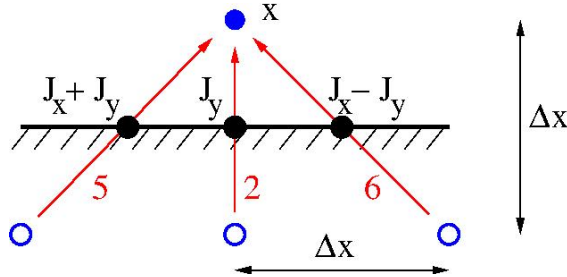


Figure 6: Approximation of the momentum gradient with finite differences.

- Gradient of equilibrium particle distributions. Now using expressions (30), (31) and (29) we obtain the following expressions for the gradient of equilibrium particle distributions :

$$(32) \quad \left\{ \begin{array}{l} \nabla f_5^{\text{eq}} \bullet (-\Delta x, -\Delta x) = \frac{1}{36} (4 + \beta + 2\alpha) (\rho(x) - \rho(x + (\Delta x, \Delta x))) \\ \quad + \frac{1}{6\lambda} [(J_x + J_y)(x - \frac{\Delta x}{2}) - (j_x(x) + j_y(x))] + O(\Delta x^2), \\ \nabla f_2^{\text{eq}} \bullet (0, -\Delta x) = \frac{1}{36} (4 - 2\beta - \alpha) (\rho(x) - \rho(x + (0, \Delta x))) \\ \quad + \frac{2}{3\lambda} (J_x(x) - j_y(x)) + O(\Delta x^2), \\ \nabla f_6^{\text{eq}} \bullet (\Delta x, -\Delta x) = \frac{1}{36} (4 + \beta + 2\alpha) (\rho(x) - \rho(x + (-\Delta x, \Delta x))) \\ \quad - \frac{1}{6\lambda} [(J_x - J_y)(x + \frac{\Delta x}{2}) - (j_x(x) - j_y(x))] + O(\Delta x^2). \end{array} \right.$$

So by using the equations (28) and (32) in the expressions given by (27) we get the following expansion of the ‘‘boundary gaps’’ :

$$\begin{aligned} b_l &\equiv f_5^*(x - (\Delta x, \Delta x)) - f_7^*(x) \\ &= \frac{1}{6\lambda} (J_x + J_y) \left(x - \frac{\Delta x}{2}\right) + \frac{1}{6} (q_x^*(x) + q_y^*(x) + \frac{1}{\lambda} (j_x(x) + j_y(x))) \\ &\quad + \frac{1}{36} (2\alpha + \beta + 4) (\rho(x) - \rho(x + (\Delta x, \Delta x))) + O(\Delta x^2), \\ b_m &\equiv f_2^*(x - (0, \Delta x)) - f_4^*(x) \\ &= \frac{2}{3\lambda} J_y(x) - \frac{1}{3} (q_y^*(x) + \frac{1}{\lambda} j_y(x)) \\ &\quad + \frac{1}{36} (-\alpha - 2\beta + 4) (\rho(x) - \rho(x + (0, \Delta x))) + O(\Delta x^2), \\ b_r &\equiv f_6^*(x + (\Delta x, -\Delta x), t) - f_8^*(x) \\ &= -\frac{1}{6\lambda} (J_x - J_y) \left(x + \frac{\Delta x}{2}\right) - \frac{1}{6} (q_x^*(x) - q_y^*(x) + \frac{1}{\lambda} (j_x(x) - j_y(x))) \\ &\quad + \frac{1}{36} (2\alpha + \beta + 4) (\rho(x) - \rho(x + (-\Delta x, \Delta x))) + O(\Delta x^2). \end{aligned}$$

Thus the result of the proposition is a direct consequence of the above expressions. \square .

4) Analysis of first order bounce back

In this section we perform a formal analysis of first order bounce back scheme (26) given in the Proposition 3. We consider here the same configuration as before (*i.e.* bottom boundary condition described in Fig. 2). In this case we give the development of the velocity on the boundary node up to order two in space in the following proposition.

Proposition 4. Expansion of the momentum for first order bounce back

We have the following expansion of momentum in the first cell up to order 2 :

$$(33) \quad \left\{ \begin{array}{l} j_x = J_x + \frac{\Delta x}{2} \partial_y J_x - 3 \Delta t \partial_t J_x - \frac{\lambda \Delta x}{4} (4 + \alpha) \partial_y \rho \\ \quad + \Delta x^2 \left[\alpha_{tt}^1 \partial_t^2 J_x + \alpha_{ty}^1 \partial_t \partial_y J_x + \alpha_{xx}^1 \partial_x^2 J_x + \alpha_{yy}^1 \partial_y^2 J_x + \beta_{tx}^1 \partial_t \partial_x J_y \right. \\ \quad \left. + \beta_{xy}^1 \partial_x \partial_y J_y + \gamma_{tx}^1 \partial_t \partial_x \rho + \gamma_{xy}^1 \partial_x \partial_y \rho \right] + O(\Delta x^3), \\ j_y = J_y + \frac{\Delta x}{2} \partial_y J_y - \Delta t \partial_t J_y - \frac{1}{6} \lambda \Delta x (4 + \alpha) \partial_y \rho \\ \quad + \Delta x^2 \left[\theta_{tx}^1 \partial_t \partial_x J_x + \theta_{xy}^1 \partial_x \partial_y J_x + \eta_{tt}^1 \partial_t^2 J_y + \eta_{ty}^1 \partial_t \partial_y J_y + \eta_{xx}^1 \partial_x^2 J_y \right. \\ \quad \left. + \eta_{yy}^1 \partial_y^2 J_y + \zeta_{ty}^1 \partial_t \partial_y \rho + \zeta_{yy}^1 \partial_y^2 \rho \right] + O(\Delta x^3). \end{array} \right.$$

with

$$(34) \quad \left\{ \begin{array}{l} \alpha_{tt}^1 = \frac{15}{2\lambda^2}, \quad \alpha_{ty}^1 = \frac{1}{4\lambda} (4\sigma_7 - 6\sigma_4 - 11), \quad \alpha_{xx}^1 = \frac{1}{24} (24\sigma_4 + 4\sigma_8 + 19), \\ \alpha_{yy}^1 = \frac{1}{4} (2\sigma_4 + 1), \quad \beta_{tx}^1 = \frac{1}{12\lambda} (12\sigma_4 - 2\sigma_8 - 11), \\ \beta_{xy}^1 = \frac{1}{12} (2\sigma_8 - 6\sigma_4 + 12), \quad \gamma_{tx}^1 = \frac{1}{12\lambda} (17\alpha + \beta - 2\beta\sigma_8 + 2\alpha\sigma_3 + 72), \\ \gamma_{xy}^1 = \frac{\lambda}{36} (88 + 28\alpha + 12\sigma_4 + 6\beta + 4\sigma_8 + 3\sigma_4\alpha + 12\alpha\sigma_7 + 12\beta\sigma_7 + \alpha\sigma_8), \\ \theta_{tx}^1 = -\frac{1}{12\lambda} (5 - 4\sigma_7 + 6\sigma_4), \quad \theta_{xy}^1 = \frac{1}{4}, \quad \eta_{ty}^1 = -\frac{1}{12\lambda} (11 + 2\sigma_4), \\ \eta_{xx}^1 = \frac{1}{24} (1 + 4\sigma_4), \quad \eta_{xy}^1 = \frac{1}{12} (5 + 2\sigma_4), \quad \zeta_{ty}^1 = \frac{1}{24} (2\alpha\sigma_3 + 16 + 3\alpha), \\ \zeta_{xx}^1 = -\frac{\lambda}{36} (-4\sigma_7 + 16 + \beta + 12\sigma_4 + 5\alpha + \alpha\sigma_7 + 2\beta\sigma_7 + 3\sigma_4\alpha), \\ \zeta_{yy}^1 = -\frac{\lambda}{72} (11 + 2\sigma_4) (4 + \alpha). \end{array} \right.$$

Proof of Proposition 4.

We use here exactly the same method as in the proof of the Proposition 1. We begin by writing the first order bounce back given by (26) for $j \in \mathcal{B} = \{5, 2, 6\}$ in the following form :

$$(35) \quad f_j^*(x, t + \Delta t) = \sum_{\ell} T_{j,\ell} f_{\ell}^*(x, t) + \xi_j(x', t),$$

where the transmission matrix T is now :

$$T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 2/3 & -2/3 & -2/3 & 2/3 & 2/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/6 & -1/6 & 1/6 & 1/6 & 2/3 & 0 & 1/3 & 0 \\ 0 & 1/6 & -1/6 & -1/6 & 1/6 & 0 & 2/3 & 0 & 1/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

and $\xi_j(x', t)$ is the given data for $j \in \mathcal{B} = \{5, 2, 6\}$:

$$(36) \quad \left\{ \begin{array}{l} \xi_5 = \frac{1}{6} \left(1 - \frac{\Delta x}{2} \partial_x + \frac{\Delta x^2}{6} \partial_x^2 \right) (J_x + J_y) \\ \quad + \frac{4 + \beta + 2\alpha}{36} \left(-\Delta x (\partial_x + \partial_y) - \frac{\Delta x^2}{2} (\partial_x + \partial_y)^2 \right) \rho + O(\Delta x^3), \\ \xi_2 = \frac{2}{3\lambda} J_y + \frac{4 - 2\beta - \alpha}{36} \left(-\Delta x \partial_y - \frac{\Delta x^2}{2} \partial_x^2 \right) \rho(x, t) + O(\Delta x^3), \\ \xi_6 = -\frac{1}{6} \left(1 - \frac{\Delta x}{2} \partial_x + \frac{\Delta x^2}{6} \partial_x^2 \right) (J_x - J_y) \\ \quad + \frac{4 + \beta + 2\alpha}{36} \left(\Delta x (\partial_x - \partial_y) - \frac{\Delta x^2}{2} ((\partial_x - \partial_y)^2) \right) \rho + O(\Delta x^3). \end{array} \right.$$

Note here that the transmission matrix T is modified to take into account the new given data ξ . Thus we can write the unified LB scheme (11) for the first order bounce back :

$$(37) \quad \left\{ \begin{array}{l} m_k(x, t + \Delta t) = (MTM^{-1}J_0)_{k,\ell} m_\ell(x, t) \\ \quad + (M_{k,\ell}U_{\ell,j}M_{j,p}^{-1}(J_0)_{p,q}) m_q(x - v_\ell \Delta t, t) + M_{k,\ell} \xi_\ell, \end{array} \right.$$

where matrices J_0 and U are given by (15) and (14) respectively.

Then as for the Proposition 1, we expand this relation for m at order 0, 1 and 2 :

$$m = m_0 + \Delta t m_1 + \Delta t^2 m_2 + O(\Delta x^3),$$

and we expand also the equation (37) at order 0, 1 and 2. At order zero, we have to solve $K m_0 = M \xi$, where the matrix K is given by $K \equiv I - M(T + U)M^{-1}J_0$:

$$K = \begin{pmatrix} 0 & 0 & \frac{1}{\lambda} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -s_3 \alpha \lambda^2 & 0 & 0 & s_3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\lambda}{3} & 0 & s_4 & 0 & 0 & 0 & 0 \\ 0 & \frac{\lambda}{3} & 0 & 0 & 0 & s_4 & 0 & 0 & 0 \\ 0 & \frac{\lambda^2(1+3s_7)}{3} & 0 & 0 & 0 & 0 & s_7 & 0 & 0 \\ 0 & 0 & \lambda^2(s_7 - 1) & 0 & 0 & 0 & 0 & s_7 & 0 \\ -\beta s_8 \lambda^4 & 0 & -\lambda^3 & 0 & 0 & 0 & 0 & 0 & s_8 \end{pmatrix}.$$

Note here that matrix K here is different from that given by (18) and is still singular. So to solve the linear system $Km = g$, we must satisfy the compatibility condition which is $g_2 - \lambda g_0 = 0$, because the first and third lines of the matrix K are proportional. The linear space $\ker K$ is generated by $\mu \equiv (1, 0, 0, \alpha \lambda^2, 0, 0, 0, 0, \beta \lambda^4)^t$. Thus the solutions of the equation $K m_0 = M \xi$ can be written as $m_0 = \rho \mu + \Sigma M \xi$ with

$$\Sigma = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/s_3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{2\lambda}{3s_4} & 0 & 1/s_4 & 0 & 0 & 0 & 0 \\ 0 & -\lambda/s_4 & 0 & 0 & 0 & 1/s_4 & 0 & 0 & 0 \\ 0 & -\frac{\lambda^2(1+3s_7)}{s_7} & 0 & 0 & 0 & 0 & 1/s_7 & 0 & 0 \\ 0 & 0 & -\frac{\lambda^2(s_7-1)}{s_7} & 0 & 0 & 0 & 0 & 1/s_7 & 0 \\ 0 & 0 & \frac{\lambda^3}{s_8} & 0 & 0 & 0 & 0 & 0 & 1/s_8 \end{pmatrix}.$$

At order zero, we get :

$$m_0 = (\rho, J_x, J_y, \alpha \rho, 0, 0, -J_x/\lambda, -J_y/\lambda, \beta \rho)^t.$$

Note here that density ρ is not fixed and (J_x, J_y) are given functions on the boundary.

Going further in the development of equation (37), we get first order. Here the compatibility condition $g_2 - \lambda g_0 = 0$ is :

$$\lambda (\partial_t \rho + \partial_x J_x + \partial_y J_y) - \left(\partial_t J_y + \frac{\alpha + 4}{6} \lambda^2 \partial_y \rho \right) = O(\Delta x).$$

The above equation is a linear combination of the equivalent equations of the internal scheme. So this condition is satisfied. At second order, the compatibility condition still has the form :

$$\lambda (\text{conservation of the mass}) - (\text{conservation of momentum along } y) = O(\Delta x^2).$$

Thus we can find the momentum development up to order two at the boundary node at the vertex x (inside the flow, located at $\Delta x/2$ of the boundary). \square

Proposition 5. Second expression of the momentum for first order bounce back

When we replace in the expansion (33) the time derivatives by their values obtained thanks to the partial equivalent equations (21), we obtain the following expansion of the value of momenta j_x and j_y at the boundary node in terms of the exact solution J_x, J_y on the boundary :

$$(38) \quad \begin{cases} j_x = J_x + \frac{\Delta x}{2} \partial_y J_x + \Delta x^2 \left[\tilde{\alpha}_{xx}^1 \partial_x^2 J_x + \tilde{\alpha}_{yy}^1 \partial_y^2 J_x + \tilde{\beta}_{xy}^1 \partial_x \partial_y J_y + \tilde{\gamma}_{xy}^1 \partial_x \partial_y \rho \right] + O(\Delta x^3) \\ j_y = J_y + \frac{\Delta x}{2} \partial_y J_y + \Delta x^2 \left[\tilde{\theta}_{xy}^1 \partial_x \partial_y J_x + \tilde{\eta}_{xx}^1 \partial_x^2 J_y + \tilde{\eta}_{yy}^1 \partial_y^2 J_y + \tilde{\zeta}_{yy}^1 \partial_y^2 \rho \right] + O(\Delta x^3). \end{cases}$$

with

$$(39) \quad \begin{cases} \tilde{\alpha}_{xx}^1 = \frac{1}{24} (8\alpha \sigma_3 - 5 - 2\beta - 4\alpha + 4\sigma_8 + 4\beta \sigma_8), & \tilde{\alpha}_{yy}^1 = -\frac{1}{4} (2\sigma_4 - 1), \\ \tilde{\beta}_{xy}^1 = \frac{1}{12} (4\alpha \sigma_3 - 2\alpha + 2\sigma_8 - 6\sigma_4 + 2\beta \sigma_8 - \beta - 1), \\ \tilde{\gamma}_{xy}^1 = -\frac{\lambda}{6} (\beta + 3\alpha \sigma_7 + 2\beta \sigma_7 + 4\sigma_7 + \alpha), & \tilde{\theta}_{xy}^1 = \frac{1}{24} (2\alpha \sigma_3 - 2 - \alpha), \\ \tilde{\eta}_{xx}^1 = -\frac{1}{24} (4\sigma_4 - 1), & \tilde{\eta}_{yy}^1 = \frac{1}{24} (2\alpha \sigma_3 - 4\sigma_4 + 2 - \alpha), \\ \tilde{\zeta}_{xx}^1 = -\frac{\lambda}{72} (8\sigma_7 + 5\alpha + 2\beta + 6\alpha \sigma_7 + 4\beta \sigma_7 + 12). \end{cases}$$

The analysis of momentum at the boundary node obtained by first order bounce back scheme proof shows that this scheme is more accurate than the simple bounce back scheme described by (9). In fact if we compare the analysis of the two schemes we see that for first order bounce back the order one terms are null (see equations (33).) Moreover we note that with the following choice of the LB parameter $\sigma_4 = \frac{1}{4}$ (*i.e.* $-\frac{1}{4} (2\sigma_4 - 1) = \frac{1}{8}$) the coefficients of $\partial_y^2 J_x$ and $\partial_x^2 J_y$ in the equations (33) are null. Thus by this choice we get a quartic value at the boundary for Poiseuille flow. This situation is not completely satisfactory and we propose in the following section to generalize the previous first order bounce back.

5) Generalized bounce back boundary scheme

Here we extend the first order bounce back scheme described by equations (26) with the aim to cancel all the second order terms in the analysis of momentum at the boundary node given by (33), allowing to get a second order bounce back scheme. Let us introduce unknown parameters a_k , a_5 , a_6 , k_x and k_y in the previous first order bounce back scheme (see equation (26)). Thus we get the following boundary scheme for bottom boundary (see Fig. 3) :

$$(40) \quad \left\{ \begin{array}{l} f_5(x, t + \Delta t) = f_7^* + \frac{1}{6\lambda} (J_x + J_y) \left(x - \frac{\Delta x}{2}, t\right) \\ \quad + \frac{a_5}{6} (q_x^* + q_y^* + \frac{1}{\lambda} (j_x + j_y)) (x, t) + \frac{k_5}{36} (\rho(x, t) - \rho(x + (\Delta x, \Delta x), t)), \\ f_2(x, t + \Delta t) = f_4^*(x) + \frac{2}{3\lambda} J_y(x, t) - \frac{a_2}{3} (q_y^* + \frac{1}{\lambda} j_y) (x, t) \\ \quad + \frac{k_2}{36} (\rho(x, t) - \rho(x + (0, \Delta x), t)), \\ f_6(x, t + \Delta t) = f_8^* - \frac{1}{6\lambda} (J_x - J_y) \left(x + \frac{\Delta x}{2}, t\right) \\ \quad + \frac{a_6}{6} (-q_x^* + q_y^* + \frac{1}{\lambda} (-j_x + j_y)) (x, t) + \frac{k_6}{36} (\rho(x, t) - \rho(x + (-\Delta x, \Delta x), t)). \end{array} \right.$$

Note here that we recover simple bounce back scheme (essentially described by equations (9)) for all the parameters equal to zero (*i.e.* $a_2 = a_5 = a_6 = a_k = k_x = k_y = 0$). If we choose all the parameters in the way proposed in relations (26), *id est* $a_2 = a_5 = a_6 = 1$, $k_2 = 4 - \alpha - 2\beta$ and $k_5 = k_6 = 4 + 2\alpha + \beta$, we recover the first order bounce back. It is possible to derive very long formal expansions of the momenta j_x and j_y in the first cell in terms of the boundary data, as in the relations (10), (22), (33) and (38).

- Analysis of the generalized bounce back

For this extended bounce back we still have the following relation as for first order bounce back :

$$(41) \quad \begin{aligned} m_k(x, t + \Delta t) &= (MTM^{-1}J_0)_{k,\ell} m_\ell(x, t) \\ &+ (M_{k,\ell}U_{\ell,j}M_{j,p}^{-1}(J_0)_{p,q}) m_q(x - v_\ell\Delta t, t) + M_{k,\ell}\xi_\ell. \end{aligned}$$

The matrix U is unchanged but the transmission matrix T satisfies :

$$T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{a_2}{3} & 0 & 1 - \frac{a_2}{3} & -\frac{2a_2}{3} & -\frac{2a_2}{3} & \frac{2a_2}{3} & \frac{2a_2}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{a_5}{6} & -\frac{a_5}{6} & \frac{a_5}{6} & \frac{a_5}{6} & 2\frac{a_5}{3} & 0 & 1 - \frac{2a_5}{3} & 0 \\ 0 & \frac{a_6}{6} & -\frac{a_6}{6} & -\frac{a_6}{6} & \frac{a_6}{6} & 0 & \frac{2a_6}{3} & 0 & 1 - \frac{2a_6}{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Now to get momentum development up to order two at the boundary node we perform as in the previous section. So we expand this relation at order 0, 1 and 2 :

$$m = m_0 + \Delta t m_1 + \Delta t^2 m_2 + O(\Delta x^3).$$

At order zero we introduce the matrix $K \equiv I - M(T + U)M^{-1}J_0$. Remark that the matrix K depends on the parameters a_2, a_5, a_6, a_k, k_x and k_y . Once again, we must solve the equation

$$K m_0 = M \xi.$$

Its solution can be written as

$$m_0 = \rho \mu + \Sigma M \xi.$$

As in the previous case we get :

$$m_0 = (\rho, J_x, J_y, \alpha \rho, 0, 0, -J_x/\lambda, -J_y/\lambda, \beta \rho)^\dagger.$$

Note that in this case the compatibility condition at second order still has the form :

$$\lambda (\text{conservation of the mass}) - (\text{conservation of momentum along } y) = O(\Delta x^2).$$

The momentum (j_x, j_y) at the vertex x located at $\Delta x/2$ can be expanded as powers of Δx . We fit the parameters to get no artefact at first order and to recover the Taylor expansion at the boundary.

Proposition 6.

Interesting choice of the parameters of the generalized bounce back

If we take the parameters of the boundary scheme (40) according to the relations

$$(42) \quad \begin{cases} a_5 = a_6, \\ k_5 = k_6 = (3\alpha + 2\beta + 4)(1 - a_5)\sigma_7 + \frac{1}{2}(3\alpha + 2\beta + 5)a_5 + \frac{1}{2}(\alpha + 4) \\ k_2 = 2(3\alpha + 2\beta + 4)(a_2 - 1)\sigma_7 - (3\alpha + 2\beta + 4)a_2 + 2(\alpha + 4), \end{cases}$$

then we get the following expansion of the momentum (j_x, j_y) near the boundary :

$$(43) \quad \begin{cases} j_x = J_x + \frac{\Delta x}{2} \partial_y J_x + (2a_5 \sigma_7 - 2\sigma_7 - 2 - a_5) \Delta t \partial_t J_x \\ \quad + \frac{\lambda \Delta x}{6} (4 + \alpha) (2a_5 \sigma_7 - 2\sigma_7 - 2 - a_5) \partial_y \rho \\ \quad + \Delta x^2 \left[\alpha_{tt}^2 \partial_t^2 J_x + \alpha_{ty}^2 \partial_t \partial_x J_x + \alpha_{xx}^2 \partial_x^2 J_x + \alpha_{yy}^2 \partial_y^2 J_x + \beta_{tx}^2 \partial_t \partial_x J_y \right. \\ \quad \left. + \beta_{xy}^2 \partial_x \partial_y J_y + \gamma_{tx}^2 \partial_t \partial_x \rho + \gamma_{xy}^2 \partial_x \partial_y \rho \right] + O(\Delta x^3), \\ j_y = J_y + \frac{\Delta x}{2} \partial_y J_y - \Delta t \partial_t J_y - \frac{1}{6} \lambda \Delta x (4 + \alpha) \partial_y \rho \\ \quad + \Delta x^2 \left[\theta_{tx}^2 \partial_t \partial_x J_x + \theta_{xy}^2 \partial_x \partial_y J_x + \eta_{tt}^2 \partial_t^2 J_y + \eta_{ty}^2 \partial_t \partial_y J_y + \eta_{xx}^2 \partial_x^2 J_y \right. \\ \quad \left. + \eta_{yy}^2 \partial_y^2 J_y + \zeta_{ty}^2 \partial_t \partial_y \rho + \zeta_{yy}^2 \partial_y^2 \rho \right] + O(\Delta x^3). \end{cases}$$

with the following coefficients for the first component :

$$\begin{cases} \alpha_{tt}^2 = \frac{1}{\lambda^2} (6\sigma_7^2 + 4a_5^2 \sigma_7^2 - 10a_5 \sigma_7^2 + 7\sigma_7 - 3a_5 \sigma_7 - 4a_5^2 \sigma_7 + \frac{5}{2} + 4a_5 + a_5^2), \\ \alpha_{ty}^2 = \frac{1}{4\lambda} (8a_5 \sigma_7 - 4\sigma_7 - 6\sigma_4 - 7 - 4a_5), \\ \alpha_{xx}^2 = -\frac{1}{24} (8a_5 \sigma_7 - 8\sigma_7 \sigma_8 + 24\sigma_4 a_5 \sigma_7 + 8a_5 \sigma_7 \sigma_8 - 8\sigma_7 - 24\sigma_4 \sigma_7 \\ \quad - 12\sigma_4 a_5 - 4a_5 - 4a_5 \sigma_8 - 15 - 12\sigma_4), \quad \alpha_{yy}^2 = \frac{1}{4} (2\sigma_4 + 1), \end{cases}$$

$$\left\{ \begin{array}{l} \beta_{tx}^2 = -\frac{1}{12\lambda} (9 + 12\sigma_4 a_5 \sigma_7 + 2a_5 + 4\sigma_7 - 4a_5 \sigma_7 + 2a_5 \sigma_8 + 4\sigma_7 \sigma_8 - 6\sigma_4 \\ \quad - 6\sigma_4 a_5 - 12\sigma_4 \sigma_7 - 4a_5 \sigma_7 \sigma_8), \\ \beta_{xy}^2 = \frac{1}{12} (12\sigma_4 a_5 \sigma_7 + 4\sigma_7 - 12\sigma_4 \sigma_7 + 4\sigma_7 \sigma_8 - 4a_5 \sigma_7 - 4a_5 \sigma_7 \sigma_8 + 2a_5 \\ \quad - 6\sigma_4 a_5 + 2a_5 \sigma_8 + 9), \end{array} \right.$$

$$\left\{ \begin{array}{l} \gamma_{tx}^2 = \frac{1}{12} (30 + 7\alpha + \beta + 8a_5^2 + 64\sigma_7 + 3\alpha\sigma_3 + 34a_5 - 32a_5\sigma_7 - 2\beta a_5\sigma_8 \\ \quad - 4\beta\sigma_7\sigma_8 - \alpha a_5\sigma_3 - 2\alpha\sigma_7\sigma_3 - 72a_5\sigma_7^2 + 40\sigma_7^2 + 2\alpha a_5\sigma_7\sigma_3 \\ \quad + 4\beta a_5\sigma_7\sigma_8 + 32a_5^2\sigma_7^2 - 32a_5^2\sigma_7 + 2\beta\sigma_7 + 17\alpha\sigma_7 - 2a_5\sigma_7\beta \\ \quad - 9\alpha a_5\sigma_7 + 8a_5\alpha + 6\sigma_7^2\alpha - 4\sigma_7^2\beta + 2a_5^2\alpha + 8a_5^2\sigma_7^2\alpha - 8\alpha a_5^2\sigma_7 \\ \quad - 14a_5\sigma_7^2\alpha + 4a_5\sigma_7^2\beta), \\ \gamma_{xy}^2 = -\frac{\lambda}{36} (60 - 6\sigma_7\alpha\sigma_4 + 2\sigma_7\alpha\sigma_8 + a_5\alpha\sigma_8 + 15\alpha + 8\sigma_7\sigma_8 + 4a_5\sigma_8 - 12\sigma_4 a_5 \\ \quad - 24\sigma_4\sigma_7 + 24\sigma_4 + 56\sigma_7 + 28a_5 - 56a_5\sigma_7 + 6\alpha\sigma_4 - 8a_5\sigma_7\sigma_8 \\ \quad + 24\sigma_4 a_5\sigma_7 + 24\beta\sigma_7 + 38\alpha\sigma_7 - 12a_5\sigma_7\beta - 26a_5\sigma_7\alpha + 6a_5\beta + 13\alpha a_5 \\ \quad - 2\alpha a_5\sigma_7\sigma_8 + 6\alpha a_5\sigma_7\sigma_4 - 3a_5\alpha\sigma_4), \end{array} \right.$$

and the coefficients for the second component given according to :

$$\left\{ \begin{array}{l} \theta_{tx}^2 = -\frac{1}{4\lambda} \frac{(4a_5\sigma_7 - 3 - 2a_5 - 6\sigma_4)(2\sigma_7 a_2 - 2\sigma_7 - a_2 - 1)}{4a_5\sigma_7 - 2a_5 + 2\sigma_7 a_2 - 6\sigma_7 - 3 - a_2}, \\ \theta_{xy}^2 = \frac{1}{12} \frac{1}{4a_5\sigma_7 - 2a_5 + 2\sigma_7 a_2 - 6\sigma_7 - 3 - a_2} (12\sigma_7 a_2 \sigma_4 - 4\sigma_7 a_2 \sigma_8 + 14\sigma_7 a_2 \\ \quad - 6\sigma_4 a_2 + 2a_2 \sigma_8 - 7a_2 + 4a_5\sigma_7 - 18\sigma_7 + 4a_5\sigma_7\sigma_8 - 12a_5\sigma_7\sigma_4 \\ \quad + 6a_5\sigma_4 - 2a_5\sigma_8 - 2a_5 - 9), \end{array} \right.$$

$$\left\{ \begin{array}{l} \eta_{ty}^2 = \frac{1}{12\lambda} \frac{1}{4a_5\sigma_7 - 2a_5 + 2\sigma_7 a_2 - 6\sigma_7 - 3 - a_2} (-26\sigma_7 a_2 + 4\sigma_7 a_2 \sigma_8 + 13a_2 \\ \quad - 2a_2 \sigma_8 + 12\sigma_4 \sigma_7 - 4a_5 \sigma_7 \sigma_8 - 12\sigma_4 a_5 \sigma_7 - 40a_5 \sigma_7 + 66\sigma_7 \\ \quad + 20a_5 + 2a_5 \sigma_8 + 6\sigma_4 a_5 + 6\sigma_4 + 33), \\ \eta_{xy}^2 = -\frac{1}{12} \frac{1}{4a_5\sigma_7 - 2a_5 + 2\sigma_7 a_2 - 6\sigma_7 - 3 - a_2} (-14\sigma_7 a_2 + 4\sigma_7 a_2 \sigma_8 + 7a_2 \\ \quad - 2a_2 \sigma_8 - 16a_5 \sigma_7 + 12\sigma_4 \sigma_7 + 30\sigma_7 - 12\sigma_4 a_5 \sigma_7 - 4a_5 \sigma_7 \sigma_8 \\ \quad + 8a_5 + 2a_5 \sigma_8 + 6\sigma_4 a_5 + 6\sigma_4 + 15), \end{array} \right.$$

$$\left\{ \begin{array}{l} \zeta_{ty}^2 = \frac{1}{24} \frac{1}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} \left(-48 - 9 \alpha - 96 \sigma_7 - 6 \alpha \sigma_3 - 24 a_2 \right. \\ \quad -24 a_5 + 64 a_5 \sigma_7 + 32 \sigma_7 a_2 + 4 \beta a_5 \sigma_8 + 2 \alpha a_5 \sigma_3 - 12 \alpha \sigma_7 \sigma_3 \\ \quad +32 \sigma_7^2 a_2 - 32 a_5 \sigma_7^2 - 4 \alpha a_5 \sigma_7 \sigma_3 - 8 \beta a_5 \sigma_7 \sigma_8 - 18 \alpha \sigma_7 + 4 a_5 \sigma_7 \beta \\ \quad +18 a_5 \sigma_7 \alpha - 6 a_2 \alpha - 2 a_2 \beta + 2 a_5 \beta - 3 a_5 \alpha - 4 \sigma_7 a_2 \beta - 8 \alpha a_2 \sigma_3 \\ \quad +24 \sigma_7^2 a_2 \alpha + 16 \sigma_7^2 a_2 \beta - 4 a_2 \beta \sigma_8 - 24 a_5 \sigma_7^2 \alpha - 16 a_5 \sigma_7^2 \beta \\ \quad \left. +8 \sigma_7 a_2 \beta \sigma_8 + 16 \alpha \sigma_7 a_2 \sigma_3 \right), \\ \zeta_{xx}^2 = \frac{\lambda}{24} \frac{1}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} \left(4 a_5 \sigma_7 \beta - 16 \sigma_7 - 8 \beta \sigma_7 - 12 \alpha \sigma_7 \right. \\ \quad \left. +10 a_5 \sigma_7 \alpha + 24 a_5 \sigma_7 - 20 - 24 \sigma_4 - 5 a_5 \alpha - 5 \alpha - 6 \alpha \sigma_4 - 12 a_5 - 2 a_5 \beta \right), \\ \zeta_{yy}^2 = -\frac{\lambda}{72} \frac{1}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} \left(-132 - 12 \sigma_7 \alpha \sigma_4 - 2 a_5 \alpha \sigma_8 - 33 \alpha \right. \\ \quad +8 a_2 \sigma_8 - 8 a_5 \sigma_8 - 24 \sigma_4 a_5 - 48 \sigma_4 \sigma_7 - 24 \sigma_4 - 264 \sigma_7 - 40 a_2 - 92 a_5 \\ \quad +208 a_5 \sigma_7 + 56 \sigma_7 a_2 + 48 \sigma_7^2 a_2 - 48 a_5 \sigma_7^2 - 6 \alpha \sigma_4 + 2 a_2 \alpha \sigma_8 \\ \quad -16 \sigma_7 a_2 \sigma_8 + 16 a_5 \sigma_7 \sigma_8 + 48 \sigma_4 a_5 \sigma_7 - 66 \alpha \sigma_7 + 24 a_5 \sigma_7 \beta + 76 a_5 \sigma_7 \alpha \\ \quad -4 a_2 \alpha + 6 a_2 \beta - 6 a_5 \beta - 29 a_5 \alpha - 24 \sigma_7 a_2 \beta - 10 \sigma_7 a_2 \alpha + 36 \sigma_7^2 a_2 \alpha \\ \quad +24 \sigma_7^2 a_2 \beta - 36 a_5 \sigma_7^2 \alpha - 24 a_5 \sigma_7^2 \beta - 4 \sigma_7 a_2 \alpha \sigma_8 + 4 a_5 \sigma_7 \alpha \sigma_8 \\ \quad \left. +12 a_5 \sigma_7 \alpha \sigma_4 - 6 a_5 \alpha \sigma_4 \right). \end{array} \right.$$

Proposition 7.

A second expression of the momenta expansion for the generalized bounce back

If we take the parameters of the boundary scheme (40) according to (42), we can drop away the unstationary terms in (43) with the help of the partial differential equations (21). Then we get the following expansion of the momentum (j_x, j_y) near the boundary :

$$(44) \left\{ \begin{array}{l} j_x = J_x + \frac{\Delta x}{2} \partial_y J_x + \Delta x^2 \left[\tilde{\alpha}_{xx}^2 \partial_x^2 J_x + \tilde{\alpha}_{yy}^2 \partial_y^2 J_x + \tilde{\beta}_{xy}^2 \partial_x \partial_y J_y + \tilde{\gamma}_{xy}^2 \partial_x \partial_y \rho \right] + O(\Delta x^3) \\ j_y = J_y + \frac{\Delta x}{2} \partial_y J_y \\ \quad + \Delta x^2 \left[\tilde{\theta}_{xy}^2 \partial_x \partial_y J_x + \tilde{\eta}_{xx}^2 \partial_x^2 J_y + \tilde{\eta}_{yy}^2 \partial_y^2 J_x + \tilde{\zeta}_{xx}^2 \partial_x^2 \rho + \tilde{\zeta}_{yy}^2 \partial_y^2 \rho \right] + O(\Delta x^3). \end{array} \right.$$

The associated coefficients are given by the following relations :

$$\left\{ \begin{array}{l} \tilde{\alpha}_{xx}^2 = -\frac{1}{24} \left(5 - 8 \sigma_7 \sigma_4 - 8 \sigma_7 \sigma_8 + 6 \alpha \sigma_7 + 4 \beta \sigma_7 - 6 a_5 \sigma_7 \alpha + 8 \beta a_5 \sigma_7 \sigma_8 + 12 \alpha a_5 \sigma_7 \sigma_3 \right. \\ \quad +4 \alpha + 2 \beta - 4 a_5 \sigma_7 \beta - 8 \beta \sigma_7 \sigma_8 + 4 \sigma_4 + 8 \sigma_7 + 8 a_5 \sigma_7 \sigma_4 + 8 a_5 \sigma_7 \sigma_8 \\ \quad -2 \alpha \sigma_3 - 8 a_5 \sigma_7 + 16 a_5 \sigma_7^2 - 16 \sigma_7^2 - 12 \sigma_7^2 \alpha - 8 \sigma_7^2 \beta - 4 a_5 \sigma_8 - 4 a_5 \sigma_4 \\ \quad \left. -4 \beta a_5 \sigma_8 + 8 a_5 \sigma_7^2 \beta + 12 a_5 \sigma_7^2 \alpha - 12 \alpha \sigma_7 \sigma_3 - 6 \alpha a_5 \sigma_3 \right), \\ \tilde{\alpha}_{yy}^2 = \frac{1}{12} \left(8 a_5 \sigma_7 \sigma_4 + 3 - 4 a_5 \sigma_4 - 2 \sigma_4 - 8 \sigma_7 \sigma_4 \right), \end{array} \right.$$

$$\left\{ \begin{array}{l}
 \tilde{\beta}_{xy}^2 = -\frac{1}{12} (1 + 12 \sigma_7 \sigma_4 - 4 \sigma_7 \sigma_8 + 3 \alpha \sigma_7 + 2 \beta \sigma_7 - 3 a_5 \sigma_7 \alpha + 4 \beta a_5 \sigma_7 \sigma_8 + 6 \alpha a_5 \sigma_7 \sigma_3 \\
 \quad + 2 \alpha + \beta - 2 a_5 \sigma_7 \beta - 4 \beta \sigma_7 \sigma_8 + 4 \sigma_7 - 12 a_5 \sigma_7 \sigma_4 + 4 a_5 \sigma_7 \sigma_8 - \alpha \sigma_3 \\
 \quad - 4 a_5 \sigma_7 + 8 a_5 \sigma_7^2 - 8 \sigma_7^2 - 6 \sigma_7^2 \alpha - 4 \sigma_7^2 \beta - 2 a_5 \sigma_8 + 6 a_5 \sigma_4 - 2 \beta a_5 \sigma_8 \\
 \quad + 4 a_5 \sigma_7^2 \beta + 6 a_5 \sigma_7^2 \alpha - 6 \alpha \sigma_7 \sigma_3 - 3 \alpha a_5 \sigma_3), \\
 \tilde{\gamma}_{xy}^2 = \frac{\lambda}{6} (2 a_5 \sigma_7 \alpha + 2 a_5 \sigma_7 \beta - a_5 \beta - 5 \alpha \sigma_7 - 4 \beta \sigma_7 - a_5 \alpha - 4 \sigma_7), \\
 \tilde{\theta}_{xy}^2 = -\frac{1}{24} \frac{1}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} \left(-6 - 6 \alpha \sigma_7 + 10 a_5 \sigma_7 \alpha - 4 a_2 \alpha \right. \\
 \quad - 2 a_2 \beta - 4 \sigma_7 a_2 \alpha - 4 \sigma_7 a_2 \beta + 2 a_5 \beta + a_5 \alpha - 4 \alpha a_2 \sigma_3 + 24 \sigma_7^2 a_2 \alpha \\
 \quad - 4 a_2 \beta \sigma_8 + 16 \beta \sigma_7^2 a_2 + 8 \alpha \sigma_7 a_2 \sigma_3 + 8 \sigma_7 a_2 \beta \sigma_8 - 4 a_2 \sigma_8 \\
 \quad - 8 \beta a_5 \sigma_7 \sigma_8 - 20 \alpha a_5 \sigma_7 \sigma_3 + 12 \sigma_4 a_2 - 3 \alpha + 8 \sigma_7 a_2 \sigma_8 + 4 a_5 \sigma_7 \beta \\
 \quad - 12 \sigma_7 - 24 \sigma_7 a_2 \sigma_4 + 24 a_5 \sigma_7 \sigma_4 - 8 a_5 \sigma_7 \sigma_8 + 6 \alpha \sigma_3 - 2 a_2 - 4 a_5 \\
 \quad + 24 a_5 \sigma_7 - 12 \sigma_7 a_2 - 32 a_5 \sigma_7^2 + 32 \sigma_7^2 a_2 + 4 a_5 \sigma_8 - 12 a_5 \sigma_4 \\
 \quad \left. + 4 \beta a_5 \sigma_8 - 16 a_5 \sigma_7^2 \beta - 24 a_5 \sigma_7^2 \alpha + 12 \alpha \sigma_7 \sigma_3 + 10 \alpha a_5 \sigma_3 \right), \\
 \tilde{\eta}_{xx}^2 = \frac{1}{24} \frac{1}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} \left(-6 \sigma_7 - 3 a_2 - 32 a_5 \sigma_7 \sigma_4 \right. \\
 \quad \left. + 8 \sigma_7 a_2 \sigma_4 - 3 + 12 \sigma_4 + 6 \sigma_7 a_2 + 16 a_5 \sigma_4 + 24 \sigma_7 \sigma_4 - 4 \sigma_4 a_2 \right), \\
 \tilde{\eta}_{yy}^2 = -\frac{1}{24} \frac{1}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} \left(6 - 24 \sigma_7 \sigma_4 - 6 \alpha \sigma_7 + 10 a_5 \sigma_7 \alpha \right. \\
 \quad - 4 a_2 \alpha - 2 a_2 \beta - 4 \sigma_7 a_2 \alpha - 4 \sigma_7 a_2 \beta + 2 a_5 \beta + a_5 \alpha - 4 \alpha a_2 \sigma_3 \\
 \quad + 24 \sigma_7^2 a_2 \alpha - 4 a_2 \beta \sigma_8 + 16 \beta \sigma_7^2 a_2 + 8 \alpha \sigma_7 a_2 \sigma_3 + 8 \sigma_7 a_2 \beta \sigma_8 \\
 \quad - 4 a_2 \sigma_8 - 8 \beta a_5 \sigma_7 \sigma_8 - 20 \alpha a_5 \sigma_7 \sigma_3 - 8 \sigma_4 a_2 - 3 \alpha + 8 \sigma_7 a_2 \sigma_8 \\
 \quad + 4 a_5 \sigma_7 \beta - 12 \sigma_4 + 12 \sigma_7 + 16 \sigma_7 a_2 \sigma_4 + 8 a_5 \sigma_7 \sigma_4 - 8 a_5 \sigma_7 \sigma_8 \\
 \quad + 6 \alpha \sigma_3 - 2 a_2 + 8 a_5 - 12 \sigma_7 a_2 - 32 a_5 \sigma_7^2 + 32 \sigma_7^2 a_2 + 4 a_5 \sigma_8 \\
 \quad \left. - 4 a_5 \sigma_4 + 4 \beta a_5 \sigma_8 - 16 a_5 \sigma_7^2 \beta - 24 a_5 \sigma_7^2 \alpha + 12 \alpha \sigma_7 \sigma_3 + 10 \alpha a_5 \sigma_3 \right), \\
 \tilde{\zeta}_{xx}^2 = \frac{\lambda}{24} \frac{2 \sigma_7 a_2 - 2 \sigma_7 - a_2 - 1}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} \left(-8 \beta \sigma_7 - 12 \alpha \sigma_7 - 16 \sigma_7 + 8 a_5 \sigma_7 \right. \\
 \quad \left. + 6 a_5 \sigma_7 \alpha + 4 a_5 \sigma_7 \beta - 3 a_5 \alpha - 2 \alpha - 4 a_5 - 2 a_5 \beta - 8 \right), \\
 \tilde{\zeta}_{yy}^2 = -\frac{\lambda}{24} \frac{(2 \sigma_7 - 1)^2}{4 a_5 \sigma_7 - 2 a_5 + 2 \sigma_7 a_2 - 6 \sigma_7 - 3 - a_2} (3 \alpha + 2 \beta + 4) (a_2 - a_5).
 \end{array} \right.$$

6) Numerical test

• Let first consider Poiseuille flow driven by a pressure gradient in the domain $\Omega = [1, N_x] \times [1, N_y]$. So we apply “anti-bounce back” boundary condition at inlet ($i = 1$) and outlet ($i = N_x$) of the channel to impose pressure δp and $-\delta p$ and simple bounce back on the bottom $j = 1$ and the top $j = N_y$ of the domain to impose $u_y = 0$. So the solid wall ($j_x = 0$) of the Poiseuille solution is exactly at $\frac{\Delta x}{2}$ for the following condition :

$$\sigma_4 \sigma_7 = -\frac{3}{8} \frac{\alpha + 4}{\alpha + 2\beta - 4},$$

as proposed in our previous contribution [2].

Now we use the extended bounce back scheme described by (40) instead of the classical bounce back to impose the homogeneous Dirichlet boundary condition $u_y = 0$. In this case

we find that the parabolic solution of the Poiseuille flow is null exactly at $\frac{\Delta x}{2}$ (*i.e.* the solid wall $j_x = 0$ is located exactly at $\frac{\Delta x}{2}$ below the first mesh vertex) for the following choice of the parameters a_5 , s_4 and s_7 :

$$(45) \quad \sigma_4 \sigma_7 = \frac{1}{16} \frac{8 a_5 \sigma_4 + 4 \sigma_4 - 3}{(a_5 - 1)}.$$

This is because when the coefficient $\tilde{\alpha}_{yy}^2$ introduced in Proposition 7 is equal to $\frac{1}{8}$, we have the relation (45). This proves numerically that this extended bounce back scheme is exact for Poiseuille flow test case. All the extra order terms of the expressions (44) are null and the developments of the j_x momentum on the boundary node becomes :

$$j_x = J_x + \frac{\Delta x}{2} \partial_y J_x + \frac{\Delta x^2}{8} \partial_y^2 J_x.$$

- We consider now the “accordion” test case introduced in our contribution [3]. In the rectangular domain $\Omega =]0, L[\times]0, h[$, we introduce periodic boundary conditions at $x = 0$ and $x = L$. For the boundaries at $y = 0$ and $y = h$, we impose $J_x(x, 0) = J_x(x, h) = J_0 \cos(2k\pi \frac{x}{L})$ and $J_y(x, 0) = J_y(x, h) = 0$, for $0 < x < L$ with the integer k equal to 1 in our simulations. In the low velocity regime the steady state is solution of the Stokes equations

$$(46) \quad \operatorname{div} J = 0, \quad -\nu \Delta J + \nabla p = 0.$$

An analytic solution is given by the following expressions. Introduce the function $f(y)$ defined by

$$f(y) = \begin{cases} -J_0 \frac{h}{\sinh(\mathcal{K} h) - \mathcal{K} h} \sinh(\mathcal{K} y) + J_0 \frac{\sinh(\mathcal{K} h)}{\sinh(\mathcal{K} h) - \mathcal{K} h} y \cosh(\mathcal{K} y) \\ + J_0 \frac{1 - \cosh(\mathcal{K} h)}{\sinh(\mathcal{K} h) - \mathcal{K} h} y \sinh(\mathcal{K} y), & \mathcal{K} = \frac{2k\pi}{L}. \end{cases}$$

The stream function $\psi = f(y) \cos(\mathcal{K} x)$, the two components $J_x = \frac{\partial \psi}{\partial y}$ and $J_y = -\frac{\partial \psi}{\partial x}$ of momentum and the pressure field $p(x, y) = \frac{\nu}{\mathcal{K}} \sin(\mathcal{K} x) (\frac{d^3 f}{dy^3} - \mathcal{K}^2 \frac{df}{dy})$ define a particular solution of the Stokes problem (46).

- We have measured the error between the measured values j_x and j_y in the first cell and the four following quantities : (i) the given value J_x and J_y on the boundary, (ii) the result of the Taylor expansion (33) taking into account only the first order terms, (iii) Taylor expansion (33) with all terms of second order and (iv) the exact values $J_x(x, \frac{\Delta x}{2})$ and $J_y(x, \frac{\Delta x}{2})$ of the problem (46) at the mesh point location.

We have done two numerical experiments. One (see Fig. 7) with very simple values of the coefficients of (40) : $a_2 = a_5 = a_6 = 0$, $k_2 = k_5 = k_6 = 0$ and the other (see Fig. 8) with the condition (42) and the choice $a_2 = a_5 = -1$, $k_2 = 4$, $k_5 = k_6 = 1$.

The results are as expected. This validates the formal expansion proposed in [3] for the analysis of the bounce back boundary condition. The error is only first order for the x component of the momentum. This is due to a particular good precision with only 16 mesh points (see Fig. 8).

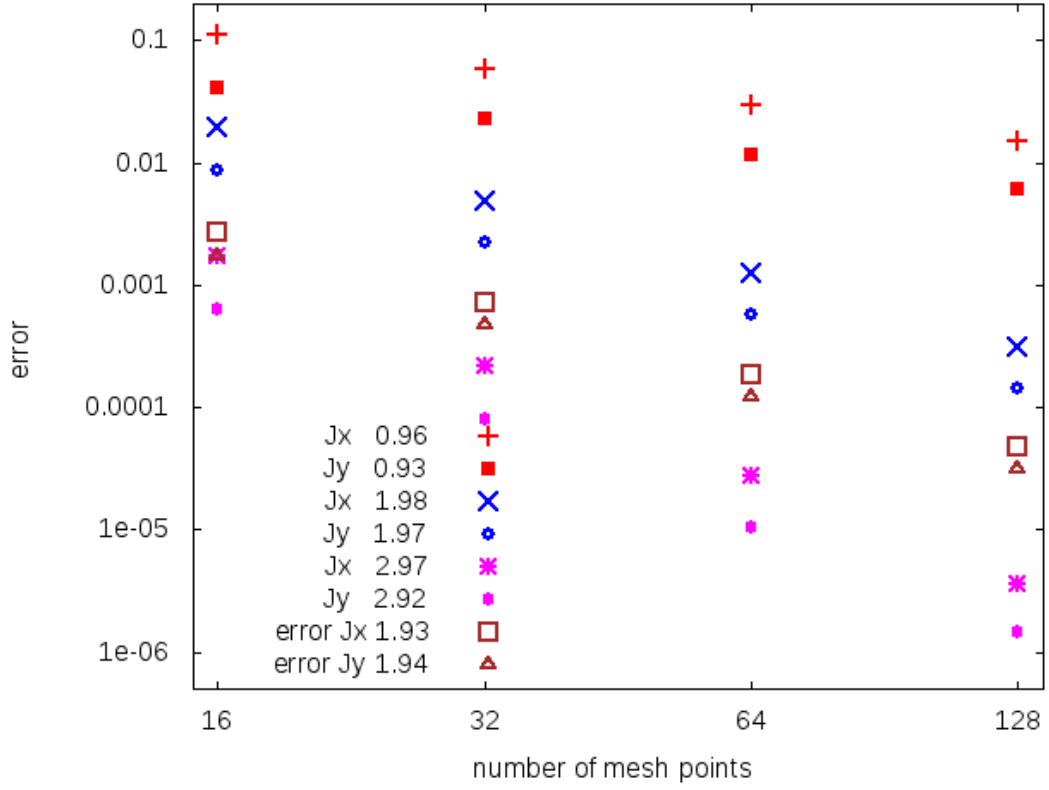


Figure 7: Theoretical and measured rates of convergence θ for classical bounce back (9) as a function of the number of mesh points in the axial direction. The error is proportional to Δx^θ in the ℓ^2 norm for x and y component of the momentum, for aspect ratio $\frac{L}{h} = 2$.

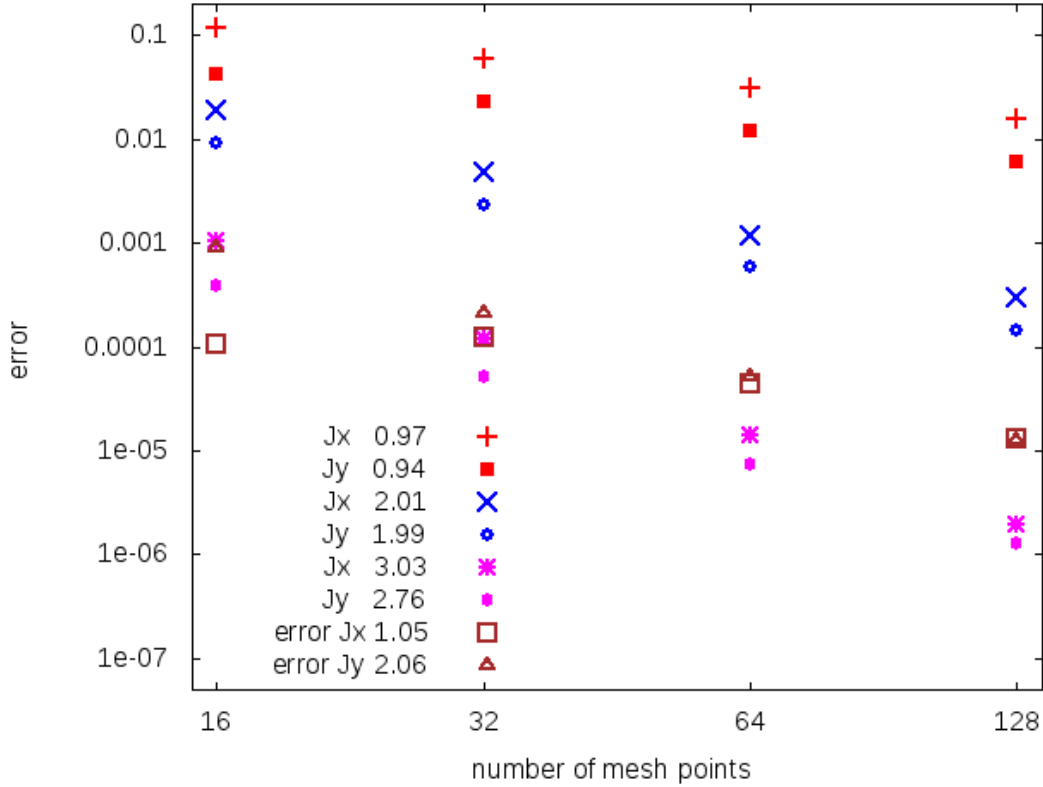


Figure 8: Theoretical and measured rates of convergence θ for generalized bounce back (40) as a function of the number of mesh points in the axial direction. The error is proportional to Δx^θ in the ℓ^2 norm for x and y component of the momentum, for aspect ratio $\frac{L}{h} = 2$.

7) Conclusion

We have shown that the classical bounce back is the result of an approximation at order zero of the internal lattice Boltzmann scheme. An analysis by an extension of the Taylor expansion method was described as in [3]. Then a new scheme called first order bounce back was proposed and analyzed. We proved that in this scheme the artefact/defect at order 1 of the classical bounce back can be removed. Finally we proposed an extended bounce back scheme where we removed all the artefacts/defects at order 1 and we proved that for a special choice the bounce back can be exact up to order two for Poiseuille flow test case. The stationary “accordion” test case shows that for a nontrivial flow, the analysis proposed for the boundary condition does not present any contradiction. Other numerical experiments will be presented in forthcoming contributions. Moreover, an analysis of the anti-bounce back [4], appropriate for taking into consideration a pressure boundary condition, seems also possible.

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