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Analysis of lattice Boltzmann boundary conditions

The correct implementation of Navier-Stokes boundary conditions in the framework of lattice Boltzmann schemes is complicated by the non-availability of analytical methods to assess the consistency of such discretizations. To close this gap, we propose a simple direct asymptotic analysis which is readily applicable to finite difference discretizations of initial boundary value problems in general and to lattice Boltzmann methods in particular. Results of the analysis applied to the classical lattice Boltzmann scheme with bounce back boundary condition are reported.

Generally speaking, the lattice Boltzmann method is a finite difference method to construct approximate solutions of the Navier-Stokes equation

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p = \nu \Delta \mathbf{v}, \qquad \mathrm{div}\mathbf{v} = 0, \qquad \text{in } \Omega \tag{1}$$

together with initial and boundary values, such as

$$\mathbf{v}(0, \mathbf{x}) = \psi(\mathbf{x}) \quad \mathbf{x} \in \Omega, \qquad \mathbf{v}(t, \mathbf{x}) = \phi(\mathbf{x}) \quad \mathbf{x} \in \partial\Omega. \tag{2}$$

In the following we consider in particular the D2Q9 lattice Boltzmann scheme as reported in [2] and we restrict ourselves to problems posed on the unit square $\Omega = [0,1]^2$. As space time grid, we choose $(t_j, \mathbf{x}_\mathbf{k}) = (h^2 j, h\mathbf{k})$ with $j \in \mathbb{N}_0$, $\mathbf{k} \in \mathbb{Z}^2$ and $\mathbf{x}_\mathbf{k} \in \Omega$. The particle population at $\mathbf{x}_k$ and t_j corresponding to velocity $\mathbf{c}_i \in \{-1, 0, 1\}^2$ is denoted $f_i(j, \mathbf{k})$. Then, the lattice Boltzmann algorithm is

$$f_i(j+1, \mathbf{k} + \mathbf{c}_i) = f_i(j, \mathbf{k}) + C_i(f)(j, \mathbf{k}) \tag{3}$$

where

$$C_i(f)(j, \mathbf{k}) = \frac{1}{\tau} \left(f_i^{eq}(\rho(j, \mathbf{k}), \mathbf{u}(j, \mathbf{k})) - f_i(j, \mathbf{k}) \right), \qquad \rho = \sum_i f_i, \qquad \mathbf{u} = \sum_i f_i \mathbf{c}_i$$

and f_i^{eq} is the equilibrium distribution reported in [2]. The initial value is assumed of the form $f_i(0, \mathbf{k}) = f_i^{eq}(1, h\psi(\mathbf{x}_\mathbf{k}))$ and at terminal nodes where a neighbor in direction $\mathbf{c}_{i^*} = -\mathbf{c}_i$ is missing, the bounce back update rule is used

$$f_i(j+1, \mathbf{k}) = f_{i^*}(j, \mathbf{k}) + C_{i^*}(f)(j, \mathbf{k}) + h\alpha_i \langle \mathbf{c}_i, \phi(\bar{\mathbf{x}}) \rangle . \tag{4}$$

Here $\alpha_i = 6 f_i^{eq}(1, 0)$, and $\bar{\mathbf{x}}$ is the closest boundary point from $\mathbf{x}_\mathbf{k}$ in direction $\mathbf{c}_{i^*}$, i.e. $\bar{\mathbf{x}} = \mathbf{x}_\mathbf{k} + q_i h \mathbf{c}_{i^*}$ with $q_i \in [0, 1)$.

In order to analyse the consistency of (3), (4) to the problem (1), (2), we follow the approach described in [5]. Specifically, we insert a regular expansion with smooth, h-independent coefficients

$$f_i(j, \mathbf{k}) = f_i^{(0)}(t_j, \mathbf{x}_k) + h f_i^{(1)}(t_j, \mathbf{x}_k) + h^2 f_i^{(2)}(t_j, \mathbf{x}_k) + \ldots \tag{5}$$

into (3) and (4). Then, we perform a Taylor expansion and equate the expressions in the different h-orders separately to zero. It turns out that the coefficients $f^{(m)}$ are completely determined by their moments

$$\rho_m = \sum_i f_i^{(m)}, \qquad \mathbf{u}_m = \sum_i f_i^{(m)} \mathbf{c}_i$$

which satisfy certain partial differential equations with initial and boundary values (see also [4] for the case of periodic boundaries). In leading order, we have

$$\nabla \cdot \mathbf{u}_0 = 0, \qquad \frac{1}{3} \nabla \rho_0 + \mathbf{u}_0 (\nabla \mathbf{u}_0) = 0, \qquad \mathbf{u}_0(0, \mathbf{x}) = 0 \quad \mathbf{x} \in \Omega, \qquad \mathbf{u}_0(t, \mathbf{x}) = 0 \quad \mathbf{x} \in \partial\Omega. \tag{6}$$

The solution of this stationary Navier-Stokes problem is given by $\mathbf{u}_0 = 0$ and $\nabla \rho_0 = 0$. As a consequence, the equations

$$\frac{\partial \rho_0}{\partial t} = \nabla \cdot \mathbf{u}_1, \qquad \nabla \rho_1 = 0, \qquad \rho_1(0, \mathbf{x}) = 0 \quad \mathbf{x} \in \Omega \tag{7}$$

imply that $\rho_0 = 1$ if $\mathbf{u}_1|_{\partial\Omega} = \phi$ and ρ_1 is a constant in space which may still depend on time. From the further condition

$$\frac{\partial \rho_1}{\partial t} = \nabla \cdot \mathbf{u}_2, \tag{8}$$

we can then conclude by integration over Ω that $\rho_1 = 0$ if $\int_{\partial\Omega} \mathbf{u}_2 \cdot \mathbf{n} = 0$. Next, the pair $\mathbf{u}_1, \rho_2$ gives rise to a solution of the Navier-Stokes problem (1), (2) upon setting $\mathbf{v} = \mathbf{u}_1$ and $p = \rho_2/3$, and $\nu = \frac{1}{3}(\tau - \frac{1}{2})$. The second order velocity $\mathbf{u}_2$ and the third order density ρ_3 satisfy a homogeneous Oseen-type equation

$$\frac{\partial \mathbf{u}_2}{\partial t} + \frac{1}{3}\nabla\rho_3 + \mathbf{u}_1(\nabla \mathbf{u}_2) + \mathbf{u}_2(\nabla \mathbf{u}_1) = \frac{1}{3}(\tau - \frac{1}{2})\triangle \mathbf{u}_2 \tag{9}$$

with initial value $\mathbf{u}_2|_{t=0} = 0$ and $\rho_3|_{t=0} = 0$. As boundary condition on $\mathbf{u}_2$, we find

$$\langle \mathbf{u}_2(\bar{\mathbf{x}}), \mathbf{c}_i \rangle = \kappa_i(1 - 2q_i) \langle S[\mathbf{u}_1](\bar{\mathbf{x}})\mathbf{c}_i, \mathbf{c}_i \rangle, \qquad \bar{\mathbf{x}} \in \partial\Omega \tag{10}$$

where $\mathbf{c}_i$ are the *incoming directions* at the boundary point $\bar{\mathbf{x}}$ and $S[\mathbf{u}_1] = \nabla \mathbf{u}_1 + (\nabla \mathbf{u}_1)^T$ is the viscous stress tensor. Finally, the equations satisfied by $\mathbf{u}_3, \rho_4$ is again of Oseen-type but now with a source term depending on the Navier-Stokes solution $\mathbf{u}_1, \rho_2$. Hence, $\mathbf{u}_3, \rho_4$ are generally different from zero so that

$$\frac{1}{h}\mathbf{u}(j, \mathbf{k}) - \mathbf{u}_1(t_j, \mathbf{x_k}) = h\mathbf{u}_2(t_j, \mathbf{x_k}) + \mathcal{O}(h^2),$$

$$\frac{1}{h^2}(\rho(j, \mathbf{k}) - 1) - \rho_2(t_j, \mathbf{x_k}) = h\rho_3(t_j, \mathbf{x_k}) + \mathcal{O}(h^2).$$

Obviously, a second order accurate velocity and 1st order pressure of the original Navier-Stokes problem are obtained with the lattice Boltzmann solution $\rho, \mathbf{u}$ if $\mathbf{u}_2$ vanishes which, in view of (9), happens when $\mathbf{u}_2(\bar{\mathbf{x}}) = 0$ for all $\bar{\mathbf{x}} \in \partial\Omega$. As examples for this situation, we mention the cases $S[\mathbf{u}_1] = 0$ on $\partial\Omega$, or $q_1 = 1/2$, i.e. all terminal nodes have distance $h/2$ from the boundary. Then (10) implies that $\mathbf{u}_2(\bar{\mathbf{x}}) = 0$ for all $\bar{\mathbf{x}} \in \partial\Omega$ because the incoming directions always include two linear independent directions. In general, however, condition (10) does not imply that $\mathbf{u}_2$ vanishes on the boundary. Worse than that, the condition (10) can typically not be satisfied at all because the left hand side of (10) is linear in $\mathbf{c}_i$ and the right hand side is quadratic! To demonstrate this problem, we consider a stationary linear Navier-Stokes flow in the unit square Ω

$$\mathbf{v}(\mathbf{x}) = A\mathbf{x}, \qquad p(\mathbf{x}) = \langle A^2\mathbf{x}, \mathbf{x} \rangle, \qquad A = \begin{pmatrix} 4 & 1 \\ 1 & -4 \end{pmatrix}. \tag{11}$$

On the right hand side of the unit square, the incoming directions are $\mathbf{c}_3 = (-1, 0)^T$, $\mathbf{c}_6 = (-1, 1)^T$, and $\mathbf{c}_7 = (-1, -1)^T$. Hence, (10) gives rise to three conditions on $\mathbf{u}_2 = (u_2^x, u_2^y)^T$

$$u_2^x = -2, \qquad u_2^x + u_2^y = -1, \qquad u_2^x - u_2^y = 1. \tag{12}$$

By adding the second and the third condition, we find $u_2^x = 0$ which obviously contradicts the first condition. This contradiction indicates that our original expansion (5) is not appropriate. In fact, from the classical theory of Boltzmann equation it is well known that rarefied gas flows typically exhibit boundary layers – so called Knudsen layers [3] – with a thickness proportional to the Knudsen number. Since the Knudsen number is coupled to the discretization parameter in the lattice Boltzmann method we expect a boundary layer of thickness $\mathcal{O}(h)$ and hence, the assumption of h-independent expansion coefficients $f^{(m)}$ is in general not sufficient to describe the numerical solution. Instead, we have to work with a more general expansion, as for example

$$f_i(j, \mathbf{k}) = f_i^{(0)}(t_j, \mathbf{x}_k) + hf_i^{(1)}(t_j, \mathbf{x}_k) + h^2(f_i^{(2)}(t_j, \mathbf{x}_k) + \tilde{f}_i^{(2)}(j, \mathbf{k})) + \ldots \tag{13}$$

where the new coefficient $\tilde{f}^{(2)}$ can incorporate the boundary layer effect (a more careful approach uses a matched asymptotic expansion to resolve the boundary layer). In any case, the additional term $\tilde{f}^{(2)}$ with moments $\tilde{\mathbf{u}}_2, \tilde{\rho}_2$ leads to

$$\frac{1}{h}\mathbf{u}(j, \mathbf{k}) - \mathbf{u}_1(t_j, \mathbf{x_k}) = h\tilde{\mathbf{u}}_2(j, \mathbf{k}) = \mathcal{O}(h),$$

$$\frac{1}{h^2}(\rho(j,\mathbf{k})-1)-\rho_2(t_j,\mathbf{x_k})=\tilde{\rho}_2(j,\mathbf{k})=\mathcal{O}(1)$$

which implies that, in general, the velocity is only first order accurate and the pressure is inconsistent when using the bounce back rule. Note that the velocity $\mathbf{u}_2$ corresponding to $f_i^{(2)}$ vanishes because it satisfies (9) with zero boundary and initial values.

To illustrate the predictions of the analysis, we apply the Lattice Boltzmann bounce back algorithm to the flow (11), i.e. we take $\psi(\mathbf{x}) = A\mathbf{x}$ and $\phi(\mathbf{x}) = A\mathbf{x}$. In figure 1, a numerical convergence analysis is given for the case $q_i = 1/2$ and $q_i = 0$.

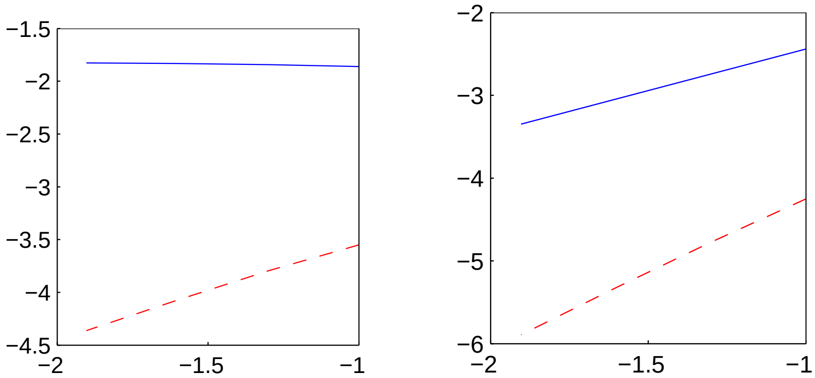

Figure 1: Double logarithmic plots of the maximal absolute error in pressure (left) and velocity (right) versus h. The solid line refers to grids with $q_i = 0$ (terminal points are located on the boundary) and the dashed line to grids with $q_i = 1/2$ (terminal points have distance $h/2$ from the boundary).

The inconsistency of the lattice Boltzmann pressure $(\rho-1)/3h^2$ can also be seen from the left part of figure 2 where a comparison with the exact pressure is shown. Note that the numerical pressure has strong gradients in the corners which indicates the non-regular behavior of $\tilde{\rho}_2$. In contrast to this, the velocity field is consistent and shows the correct behavior.

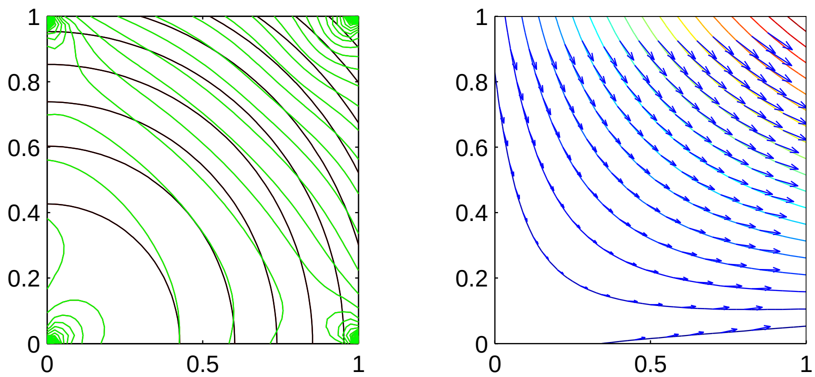

Figure 2: Left: isolines of the lattice Boltzmann pressure $(\rho-1)/3h^2$ (green) versus isolines of the exact pressure (black). Right: the lattice Boltzmann velocity is identical to the exact velocity within plotting accuracy.

An inspection of the numerical error $(\mathbf{u}/h - \mathbf{u}_1)/h$, which coincides in leading order with $\tilde{\mathbf{u}}_2$, shows the predicted boundary layers (figure 3).
We close our discussion of the bounce back condition with the remark that the asymptotic analysis can also be used constructively. Once the condition (10) has been identified as source for the unwanted term $\tilde{f}^{(2)}$, this knowledge can be used to improve the bounce back rule simply by subtracting the expression

$$f_i(j+1,\mathbf{k}) = f_{i^*}(j,\mathbf{k}) + C_{i^*}(f)(j,\mathbf{k}) + h\alpha_i\left\langle \mathbf{c}_i, \phi(\bar{\mathbf{x}})\right\rangle - h^2\kappa_i(1-2q_i)\left\langle S[\mathbf{u}_1](\bar{\mathbf{x}})\mathbf{c}_i, \mathbf{c}_i\right\rangle.$$

With a suitable discretization of the derivatives in $S[\mathbf{u}_1]$, this boundary scheme leads to a second order accurate velocity and first order accurate pressure. The same accuracy is also obtained with the method reported in [1]. The

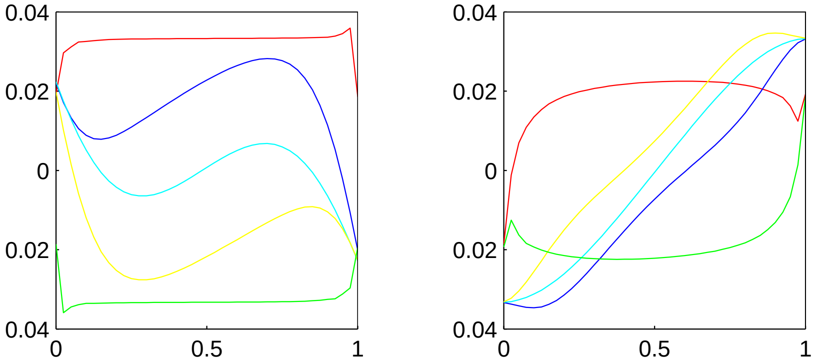

Figure 3: Components of the velocity error along several cuts in the domain. Left: x-component along cuts in y-direction. Right: y-components along cuts in y-direction.

analysis proceeds along the same lines as outlined above. Details will be given in a forthcoming paper.

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