Master's Thesis

Study of Lattice Boltzmann Boundary Conditions for Fluid Structure Interaction

Student
Andrés Mauricio Aguirre Mesa

Responsible professor
Manuel Julio García Ruiz

Department of Mechanical Engineering
Universidad EAFIT
Medellín

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Abstract

Lattice Boltzmann is a numerical method for the simulation of different physical phenomena, such as incompressible flow. Despite the fact of being a kinetic method, and therefore of unsteady nature, allows to obtain the solution of steady problems with good accuracy and efficiency. However, the arising of pressure oscillations during the solution process and the reflective character of some of its boundary conditions have resulted in an active research interest on open boundaries, and outlet conditions in particular.

Fluid structure interaction problems are mostly of unsteady type, so the elimination of spurious pressure oscillations is desirable or even necessary. The aim of the present work is to show, in the first place, that oscillations occur even without involving solid obstacles in the simulations, although measures to avoid them are taken, like diffusive scaling. On the other hand, that oscillation-free results are possible to be obtained using the most basic formulation of the method, LBGK, and even conventional reflective conditions, but sacrificing the most widely used tool of the LBM method: the bounce back condition.

Keywords: Lattice Boltzmann Method, Fluid Structure Interaction, Open Boundary Conditions, Wave Reflection.

Contents

Chapter 1

Introduction

Lattice Boltzmann is a numerical method for the solution of transport phenomena problems, based on the Boltzmann equation and the kinetic theory of gases. In spite of not being as well known as the finite element method or the finite volume method, its ability to adapt to complex geometries and being highly parallelizable make of lattice Boltzmann a very appealing method for applications such as simulation of blood vessels and flow through porous media.

It is desired to use the lattice Boltzmann method for fluid structure interaction applications by coupling it, for example, to the fixed grid finite element method. To accomplish this, two verifications are required: *(i)* to check if LBM is capable of simulating unsteady flows, and *(ii)* to check if LBM can interact with curved and mobile boundaries.

Despite the fact of being a kinetic method, and therefore having and unsteady nature, LBM has been successfully used since by its creation, 1988, to obtain steady state solutions to fluid mechanics problems. The emergence of pressure oscillations were considered for so long as "a convergence process", and this is attributed to the small compressibility of the method and the reflective character or its conventional boundary conditions.

Most of the problems related to fluid structure interaction have unsteady nature, for example, airfoil vibration induced by flow, or deformation of blood vessels under pulsatile flow, where fluid domain is continuously disturbed and it is desirable to know the evolution of force values on the interface. Therefore, the elimination of numerical perturbations is necessary in order to study physical phenomena.

There are several proposals to fix the oscillation issues, such as the use of a diffusive scaling to simulate an incompressible fluid, the domain initialization to avoid the so called "initial layers", and the development of non reflective boundaries.

In order to accomplish the first aim of this project several numerical tests were carried out, moving step by step from the solution of a simple problem, the Poiseuille flow, to the movement of a curved object inside a fluid domain. During the tests multiple boundary conditions were compared, and it was note that, although measures to avoid oscillations were taken, even applying those measures combined did not remove the oscillations.

On the other hand, a haphazard attempt to verify what happens when wall boundary conditions are ignored, by canceling the streaming step, resulted in the completely elimination of the perturbations, despite the fact that reflective boundary conditions were used for input and output, the Zou and He conditions. Moreover, the ignored condition is considered one of the cornerstones of the lattice Boltzmann method: the bounce-back condition.

Chapter 2

Literature review

The next review is conducted with the aim of verifying the advances that have been made with regard to Fluid Structure Interaction involving the Lattice Boltzmann Method, so that useful information can be obtained for subsequent proposals and developments in this topic. This chapter is structured as follows.

In the first section the current relevance of the topic is verified in terms of research interest. This is done through the quantification of the annual production, looking for a trend line that indicates whether the interest in the subject is raising or declining. It is also verified if the particular production in the theoretical or the applied field remains to be interesting for research in the present topic.

In the second section a classification of the different types of approaches used to solved FSI problems is conducted. In particular, there is an interest in verifying the scope of the different solution alternatives to model rigid or flexible fluid-solid interfaces, in order to find the most competitive alternatives.

The third section focuses on the selection of adequate straight boundary conditions for the simulation of FSI using LBM. Straight boundaries refer to boundaries that are horizontally or vertically alligned to the lattice, including openings and walls, and they are considered adequate when they allow to reach a solution without disturbing the fluid domain, for example, by the reflection of pressure waves.

Finally, some concluding remarks are set out.

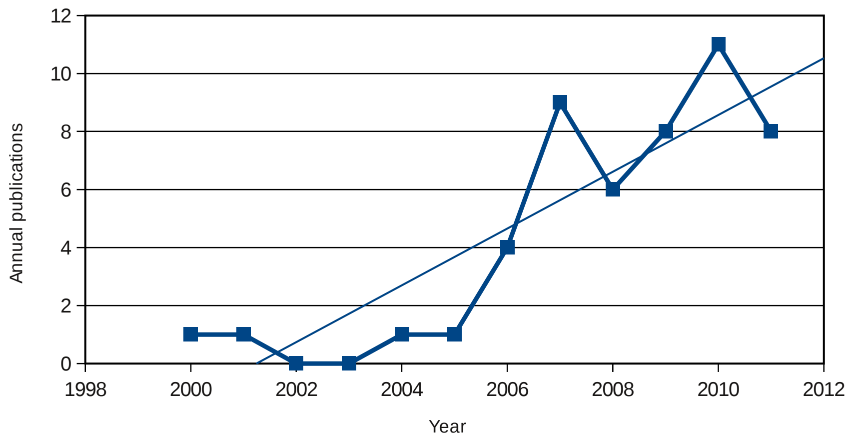


Figure 2.1: Annual publications on FSI related LBM implementations

2.1 Current relevance of the topic

The review process began by searching publications in academic databases, primarily Scopus, and Google Scholar in a lesser extent. The main search consisted in finding documents whose title, abstract, full-text or keywords contained both "fluid structure interaction" and "lattice Boltmann" terms. The evolution of publications per year according to the above criteria is summarized in figure 2.1.

Despite the fact that the annual bibliographical production presents some oscillations, it is observed a rising interest tendency about this topic. Therefore, new publications involving the lattice Boltzmann method in Fluid Structure Interaction problems are expected.

While the distinction between a theoretical paper and an applied one can be relative, for the purposes of this review the applied term refers to such publications that explicitly specify which industry or which specific problem they are focusing, and a theoretical publication concerns the development of new methods or the modification of the existing ones.

In regard to publications that focus on evaluating benchmarks, it should be noted that they are performed to measure the accuracy and stability of the evaluated methods, in order to improve them or to assess its feasibility of implementation. Due to the above, those publications have been taken into account as theoretical.

It can be seen in figure 2.2 that the production on the subject was theoretical until beyond the middle of the last decade, and thereafter study cases began to be published.

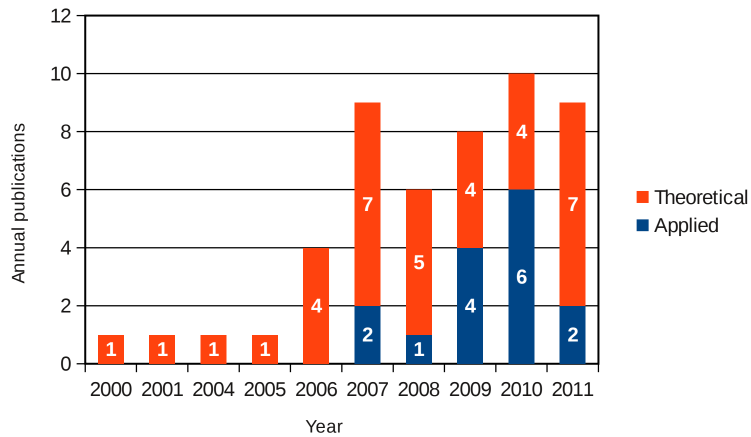


Figure 2.2: Theoretical vs applied publications

The above does not mean that developments prior to 2007 were detached from a practical purpose, given that since Krafczyk et al. (2001), the LBM was intended to simulate artificial heart valves. It appears that the method first required to tune its stability and accuracy in order to be used in problems involving fluid and solid interaction, which is the case in Breuer et al. (2000), or its jointly utilization with other methods, like in Feng and Michaelides (2004).

As related in Succi (2008), LBM has been evolving for being used in applications such as the modeling of turbulent flows and fluid structure interactions at microscopical level. Among the applications reviewed by the author, it is worth to mention the study of slip boundary conditions of the fluid particles on the wall, or *slip-motion*, which can not be explained by the basic principles of fluid mechanics based on continuum media. The author mentions that the phenomenon can be observed making the proper tuning of the LBM, rather than imposing it macroscopically.

2.2 Interface modeling scope

The methods involving FSI and LBM, depending on the target application, may have rigid or flexible fluid-solid interface. Some applications that can be found about this topic are, for example, particles and solid transport, external flow and porous media, for both types of the aforementioned interfaces. It can be observed in figure 2.3 that before 2005 the LBM had been only proposed for rigid interface problems. Studies on flexible interfaces began to be published since that year, and to date the total number of publications on

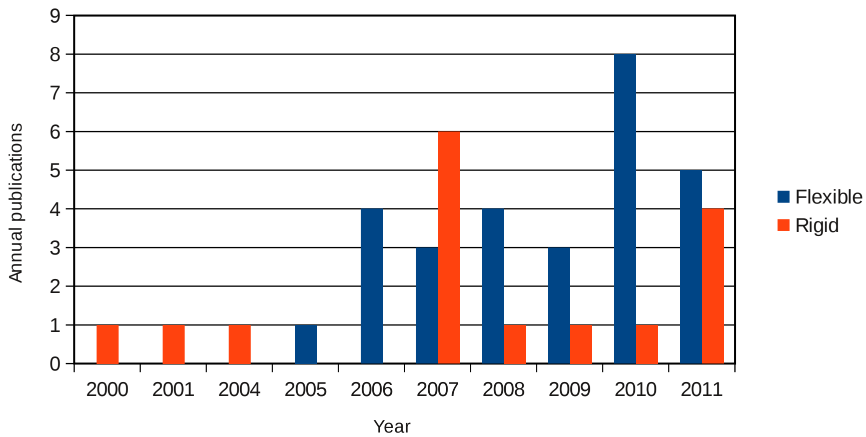


Figure 2.3: Interface modeling scope of the publications

this topic almost double the quantity of material related to rigid interfaces.

Several approaches have been used to address these problems, both monolithic and partitioned. Table 2.1 summarizes the scope of each solution approach, and the description of each one is presented next.

2.2.1 Monolithic approach using LBM

This solution alternative has one of the top places of utilization among the references found (25%). It is important to remark that the present approach have been used exclusively for solving rigid interface problems. However, it was the first that aimed to solve a practical problem, namely the simulation of artificial heart valves, which was the proposal of Krafczyk et al. (2001).

By 2001, when this solution alternative was proposed, it presented serious limitations for the solution of FSI problems, since it required a larger amount of machine resources than problems without solid domain and, in addition, this increased the chances of instability.

Despite the above, the monolithic approach is still being used in bioengineering applications, such as the aortic prosthesis design in Pelliccioni et al. (2007, 2008), in which the improvements made to the LBM are exploited, like the local lattice refinements that are possible through the use of Multiple Relaxation Times (MRT).

This approach is still subject of theoretical studies, for example, the verification of its performance in comparison with other solutions, such as the finite volume method in

Approach	Interface		Total
	Rigid	Flexible	
LBM (Monolithic)	11	0	11
DEM	4	0	4
DLM/FD	0	2	2
FDM	0	1	1
FEM	0	12	12
FG-FEM	0	1	1
IBM	1	4	5
Lattice Spring Model	0	2	2
LBFPM	0	1	1
p-FEM	0	4	4
Total	**28**	**16**	**44**

Table 2.1: Solution approaches for the solid domain

Breuer et al. (2000), and the validation of its ability to reproduce vorticity phenomena caused by external flow over fixed solid boundaries, like in Cheng et al. (2007), or moving boundaries, like the works of Geveler et al. (2011b) and Sewatkar et al. (2011).

Regarding improvement of the method, it is remarkable the proposal made in Strack and Cook (2007) on a new immersed boundary condition for moving solids. Furthermore, improvements to the accuracy and efficiency of the momentum exchange algorithm have been proposed in Caiazzo and Junk (2008) and Lorenz and Hoekstra (2009). This algorithm is responsible of the force application on the solid boundaries, and this last enhancement also seeks to preserve the Galilean invariance of the system.

The interest in this alternative remains today, as it is demonstrated in Götz et al. (2010) and Geveler et al. (2011a), where the approach is used in high performance computing.

2.2.2 DEM partitioned approach

The alternative of coupling LBM with the Discrete Element Method (DEM) shares with the monolithic approach the limitation of being used exclusively for rigid interfaces. 9% of the cases found correspond to this solution alternative, and all of them are theoretical.

Despite being used exclusively for rigid particles transport, this alternative is interesting because it incorporates the Smagorinsky turbulence model for Large Eddy Simulations (LES), supports the use of irregular boundaries and may be used for relatively high Reynolds numbers, of about 56,000, as demonstrated in Han et al. (2007a,b) and Feng et al. (2007).

Recently the method has been evaluated in Owen et al. (2011) to be used in three dimensions, also seeking to reduce their computational costs and to work with larger fluid domains than those studied so far with this alternative.

2.2.3 FEM partitioned approach

In spite of being the most widely used alternative solution (30% of the cases found), its first emergence was delayed compared to other approaches, like the IBM approach. Apparently the first proposal for the solution of the solid domain using FEM came in 2006, when Kwon (2006) proposes to alternate a LBM solver for the fluid domain and a FEM solver for the solid through the interface boundary conditions.

The author has also proposed different improvements to the approach, such as the possibility to connect the solid domain with a mismatching fluid mesh (Kwon, 2008), coupling LBM with three dimensional beam elements (Kwon and Jo, 2008a), and the development of the weighted residual based method for irregular fluid domain geometries (Kwon and Jo, 2008b, 2009).

Sui et al. (2008) proposed the use of a similar alternative for the simulation of deformable rigid bodies that travel through a fluid flow: each solid is modeled as a liquid filled capsule with a solid and flexible membrane, and the mesh can be refined in the vicinity of the interface. This proposal can be applied in cell biology and the pharmaceutical industry.

More recently, an improvement of the method was proposed using boundary tracking (front-tracking method) and it is implemented in three dimensions. In addition, it manages to relax a restriction that required the same viscosity for internal and external fluid (Sui et al., 2010). Other important theoretical developments include the implementation of the immersed boundary scheme for the solid movement (JiSeok and SangHwan, 2011), and the development of a method to simulate deformable porous media (Khan and Aidun, 2011).

Another proposal that can be applied to bioengineering is reported in Kreissl et al. (2010, 2011): the topology optimization of deformable channels, which are capable of large-scale elastic deformations at microfluidic level. It seeks to optimize the thickness distribution of active material for internal actuation and the support conditions using a nonlinear FEM solver. It is aimed at applications with low speeds and pressures, where the structural deformations caused by the fluid can be neglected, as those caused by external loads are considerably higher. According to the authors, this is a little-studied topic.

As a final application of this approach, the evaluation of hood flutter on cars and trucks is presented. The term refers to vibrations on the hood caused by air currents loading on the road. The phenomenon occurs with increasing frequency, since the new models of vehicles require increasing reductions in body weight (Gupta et al., 2009; Gaylard et al., 2010).

2.2.4 IBM partitioned approach

Since its creation by Peskin in 1970, the Immersed Boundary Method (IBM) was created specifically for FSI application, namely, modeling the flow of the blood inside the heart, which was represented by moving boundaries (Feng and Michaelides, 2004). The IBM was also the first method to be used in conjunction with LBM for FSI problems. 11% of reviewed publications use this solution alternative.

The first proposal for coupling IBM and LBM was carried out by Feng and Michaelides (2004), which uses a Lagrangian grid to follow the solid particles. The method initially presented worked for rigid solids only. This was accomplished using a penalty method, which assumes that the particle is deformable but has a very high stiffness. However, the author states that the method is easily applicable to deformable solids .

The method was improved by Sui et al. (2007), who added the capability of refining the mesh near the fluid-solid interface, and demonstrated that the approach is able to simulate the interaction of viscous flows with moving boundaries. More recently, Hao and Zhu (2010) proposed the use of implicit time steps, i.e, to calculate the interface forces of the unknown configuration for each time step. This preserves the stability of the method for longer time steps than those achieved with the explicit IBM.

The partitioned IBM-LBM approach continues being developed for medical and bio-engineering applications, as it can be seen in the works of Cheng between 2010 and 2011 (Cheng and Zhang, 2010; Cheng et al., 2011): it is used to simulate the mitral valve of the heart. It is worth mentioning that these simulations use regular Cartesian grids for the solution of the solid domain, i.e, they use fixed grids.

2.2.5 p-FEM partitioned approach

A joint solution of the LBM coupled with a High Order FEM solver (p-FEM) began to be developed in Germany by Kollmannsberger et al. (2006), who were looking for an explicit coupling of both solvers, in order to simulate vibrations on an geometrically non-linear structure caused by a Newtonian incompressible fluid. This coupling is achieved through the use of a fixed Cartesian grid, which can be even refined near the solid interface if it is required (Kollmannsberger et al., 2009). At the beginning a flag-like structure was used to verify the method, but more recently in 2010, the approach has been verified for rigid-body motion and deformation of a three dimensional immersed plate (Geller et al., 2010).

2.2.6 Other partitioned approaches

Among the least explored approaches, but not less interesting, there is the work done by Garcia et al. (2011), which uses Fixed Grid FEM to solve the solid domain. In a similar way to the proposed approaches that use p-FEM or IBM, this alternative uses a fixed Cartesian grid, which is shared by the solid and the fluid domains. It also uses the level set technique to determine the position of the solid boundary at any time.

So far the method has been tested successfully for two-dimensional external flow on both rigid and deformable solids, but the approach has not yet been developed for three dimensional flows, nor have implemented local grid refinements. For all the foregoing, the FG-LBM is a very interesting approach for future developments.

Another not so explored proposal was carried out by Shi and Phan-Tien in 2005, using the Distributed-Lagrange Multiplier / Fictitious Domain method (DLM/FD). This method uses a fixed Cartesian grid for the fluid, but not for the solid, which formulation is Lagrangian. The author state that the use of this method eliminates the need for remeshing, as would be required in an ALE formulation. The improvement of the method for three dimensional applications was developed by Shi and Lim (2007). This solution alternative has been tested successfully using the circular cylinder and the flexible plate benchmarks.

Among the alternatives found, it is noteworthy that some of them make use of mesoscopic methods for the solution of the solid domain. At one side is the proposal made in Alexeev et al. (2006) and Verberg et al. (2006), which makes use of a method called Lattice Spring Model. It have been used to simulate the movement of nanoparticle-filled microcapsules through a fluid flow. On the other side is the approach proposed by Qi et al. (2010), which makes use of the Lattice Boltzmann Flexible Particle Method (LBFPM). This method describes a solid object as a chain of rigid beam elements, which are connected by ball and socket joints. This alternative was used for the simulation of the external flow over an airfoil.

Finally, the proposal made by Ricardo Da Silva et al. (2007), contrary to other approaches, aims to a flexible boundary problem in its first publication. The method used to solve the solid part was the classic Finite Difference Method, and it is applied to single reed mouthpieces, which are characteristic parts of instruments like saxophone or clarinet.

2.3 Straight boundary conditions for unsteady problems

Works presented in this section may be valuable not only for FSI problems, but in general to unsteady CFD problems using LBM. Most of the FSI problems are unsteady in nature, and pressure oscillations issues are attributed to unadequate boundary conditions. Many of the works in this respect focus on the development of new open boundaries, but they often do not consider walls as a source of disturbances.

Some boundary conditions proposed to avoid the pressure reflection effect are the convective of the distribution functions (Yu et al., 2005), zero normal-stress, Neumann, do-nothing (Junk and Yang, 2008), characteristic non-reflecting for open boundaries (Izquierdo and Fueyo, 2008) and the convective condition of velocity (Yang, 2013).

While all aforementioned authors use vortex generation benchmarks to verify their proposals, only Izquierdo and Fueyo and Yang consider a simpler case: a 2D Poiseuille flow. However, the results of these cases are presented as normalized mass balances that do not make clear whether the pressure oscillations decrease or not. On the other hand, Kim et al. (2008) claim that the reflective effects from wall bounday conditions are not negligible, so they propose a boundary condition for both opening and wall boundaries, and their results show a clear pressure wave reduction.

Despite the importance of this topic for the spreading of lattice Boltzmann method as an efficient CFD solver, it apparently does not get enough attention and is still an active research topic, or so suggests the fact that Kim et al., having good results for the simulation of unsteady flows with LBM, has only been cited twice by January 2014[1].

2.4 Concluding remarks

- A general review of the literature on the topic studied, Fluid Structure Interaction involving Lattice Boltzmann Method, allows the observation of a growing trend in the number of publications made per year. Regarding other topics of investigation in the field of numerical methods, the present theme is a not so explored area, opening roots for new publications. It is also noted that the growing trend is present in both theoretical and applied fields.

- Research related to simulating flexible fluid-solid interfaces have appeared a little late with regarding those involving rigid interfaces. While it is early to ensure a trend for the latter, in the case of the former there is a trend of increasing interest. In particular, publications of approaches that can evaluate both type of interfaces were found, like LBM partitioned approaches with FG-FEM, p-FEM and IBM.

- Approaches that limit its scope to the solution of rigid type interfaces were also found, like monolithic LBM and partitioned coupling with DEM. A flexible interface problem can be addressed by any of the other alternatives presented here.

- Three interesting approaches to solve a FSI problem that implies large-scale deformations of the solid domain are, once again, partitioned approaches that make us of FG-FEM, p-FEM or IBM. This is due to their capability to solve the solid domain using a fixed Cartesian grid. Furthermore, each one of them is able to solve rigid interface problems, making them the most complete solution alternatives among the other approaches presented in this chapter.

- A particularly interesting approach to be studied is the one that uses Fixed Grid FEM, because it still have not been developed to simulate three dimensional cases,

[1] Checked at Scopus (www.scopus.com)

and is not yet able to make local refinements of the grid.

- Non-reflective straight boundaries is an active and not so explored topic of the lattice Boltzmann method, which is very important to efficiently simulate unsteady flows, and hence fluid structure interaction problems.

Chapter 3

Lattice Boltzmann Method for Fluid Structure Interaction

3.1 Fundamentals

The method used in the present work for the solution of the fluid domain is a standard lattice Boltzmann method with single relaxation time (LBGK) (Qian et al., 1992), using a D2Q9 lattice, which means two dimensions and nine velocities, as shown in figure 3.1.

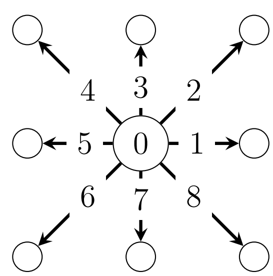


Figure 3.1: D2Q9 lattice velocities

In order to understand what lattice Boltzmann is and how it works, it is necessary to conceive a fluid from the perspective of statistical physics and the kinetic theory of gases: matter contained into a fluid domain is not a continuum nor discrete, but something in between. I.e, it can't be ignored the particle nature of matter, as it can be done by finite element method (continuum assumption), but those particles neither can't be counted or identified, as is the case of SPH method.

From the point of view of statistical physics, a fluid domain has so many particles that they are not considered countable, but they can be grouped into populations, so their macroscopic properties can be estimated statistically. Density, for example, is the mass of a particle population, contained into a very small volume.

Particle dynamics are also estimated through distribution functions f, each one defined as the probability that a part of a particle population is traveling through certain direction. That probability is expressed in mass terms, and so the summation of distribution functions for a single point of the domain is equal to the density of that point.

The lattice, which is made up by nodes and links, impose restrictions to particle populations: in terms of space, they only can be found in the nodes, and they are only able to travel in a predefined number of directions, which are represented in equations by subindex i.

Lattice directions are often called velocities, due to the fact that they depict the distance traveled by a group of particles between neighbor nodes each time step. The convention adopted in this document for the numbering of the velocities of the D2Q9 lattice was already shown in figure 3.1.

Concerning computational efficiency, physical quantities of the method are often expressed as dimensionless: lattice spacing Δx and the duration of each time step Δt are unary, then lattice velocities can only take the values $\{-1, 0, 1\}$ in either direction (equation 3.1). Consequently, other physical quantities, like pressure, velocity or force, will be dimensionless too.

$$\boldsymbol{e}_i = \begin{cases} \frac{\Delta x}{\Delta t}[0,0] & i = 0 \\ \frac{\Delta x}{\Delta t}\left[\cos\frac{\pi}{4}(i-1), \sin\frac{\pi}{4}(i-1)\right] & i = 1,3,5,7 \\ \sqrt{2}\frac{\Delta x}{\Delta t}\left[\cos\frac{\pi}{4}(i-1), \sin\frac{\pi}{4}(i-1)\right] & i = 2,4,6,8 \end{cases} \tag{3.1}$$

It is well known among experienced users of LBM, although not often referred in literature, that the relationship between lattice units and physical units is established by the law of dynamic similarity (Wolf-Gladrow, 2000). Reynolds number is enough for the scope of this work. However, it is worth mentioning that a good understanding of the studied phenomenon is very important in order to choose an adequate set of dimensionless parameters (Cates et al., 2005).

Equation 3.2 contains the expressions for converting the macroscopic quantities from lattice to physical units (Asinari et al., 2012). The r subindex stands for "real" physical units. ρ_0 is an arbitrary reference density.

$$\boldsymbol{u}_r = \boldsymbol{u}\frac{\Delta x_r}{\Delta t_r} \qquad ; \qquad P_r = [c_s^2(\rho - \rho_0)]\rho_r \left(\frac{dx_r}{dt_r}\right)^2 \tag{3.2}$$

Lattice Boltzmann is a numerical method based on the Boltzmann equation, which simulates a gas that is confined into a lattice. Particle populations can move across the lattice from node to node using lattice links, but some of them can be affected by particles that collide and change their directions. The governing equation is presented in 3.3, followed by the expressions used for the computation of the macroscopic quantities, mass density (ρ) and velocity ($\boldsymbol{u}$), which are shown in 3.4 (Chen and Doolen, 1998).

$$f_i(\boldsymbol{x} + \boldsymbol{e}_i\Delta t, t + \Delta t) = f_i(\boldsymbol{x}, t) - \frac{1}{\tau}[f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)] \tag{3.3}$$

$$\rho = \sum_i f_i \qquad ; \qquad \rho\boldsymbol{u} = \sum_i f_i\boldsymbol{e}_i \tag{3.4}$$

With the aim of simplify the programming and understanding of the method, lattice Boltzmann equation is split into two steps: collision and streaming. Collision stage (eq. 3.5) deals with the momentum exchange between particle populations occurring at each node: some particles entering a node through all its lattice links can collide and change its output direction.

$$f_i^{out}(\boldsymbol{x}, t) = f_i^{in}(\boldsymbol{x}, t) - \frac{1}{\tau}[f_i^{in}(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)] \tag{3.5}$$

It is assumed that each node of the lattice will eventually approach local thermodynamic equilibrium. Therefore, collision equation involves the equilibrium distribution function f_i^{eq}, and a temporal term τ known as relaxation time. The equilibrium distribution function and the weights that are associated to D2Q9 lattice are shown in 3.6 and 3.7 respectively (Qian et al.).

$$f_i^{eq} = t_i\rho\left[1 + 3\,\boldsymbol{e}_i \cdot \boldsymbol{u} + \frac{9}{2}(\boldsymbol{e}_i \cdot \boldsymbol{u})^2 - \frac{3}{2}\boldsymbol{u} \cdot \boldsymbol{u}\right] \tag{3.6}$$

$$t_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1,3,5,7 \\ 1/36 & i = 2,4,6,8 \end{cases} \tag{3.7}$$

The streaming stage of the LBM is responsible of spreading the mass and momentum information of the distribution functions across the lattice, simulating the movement of particle populations: a portion of the particles found in the node $\boldsymbol{x}$ at time t, which is going outside through direction i, travels through a lattice link an enters a neighbour node at time $t + \Delta t$ (eq. 3.8).

$$f_i^{in}(\boldsymbol{x} + \boldsymbol{e}_i \Delta t, t + \Delta t) = f_i^{out}(\boldsymbol{x}, t) \tag{3.8}$$

The capability of simulating an incompressible fluid with LBM is guaranteed by the *diffusive scaling*, which is a proportionality relation between the characteristic length N and characteristic time Nt of the simulation, both expressed in lattice units. According to diffusive scaling, the relation between those parameters should be: $Nt \sim N^2$. This proportionality allows the recovery of the incompressible Navier Stokes equations by an asymptotic expansion of the lattice Boltzmann equation (Junk et al., 2005).

Special care must be taken with the definition of the initial and boundary conditions of the method, due to the fact that the governing variables are distribution functions instead of macroscopic quantities. Not doing this results in the arising of spurious initial and boundary layers, which produce noise and oscillations that can affect the convergence rate and the results (Caiazzo, 2007).

3.2 Opening boundary conditions

3.2.1 Zou and He conditions

Lattice Boltzmann, as well as other compressible and pseudo-compressible methods used for CFD simulation, suffers from a pressure wave reflection effect, caused by inappropriate opening boundary conditions. This also affects the accuracy of results and the convergence rate, even for low Reynolds simulations. The boundary conditions proposed by *Zou and He* are an example of reflective boundaries (Izquierdo et al., 2009).

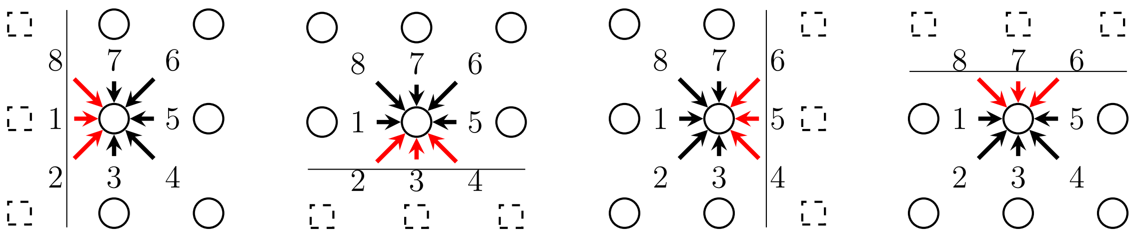


Figure 3.2: Incoming distribution functions overwritten by the Zou and He conditions, for each boundary position.

The Zou and He conditions are intended to fix the pressure or the velocity at the boundaries, computing only the distribution functions that can't be streamed, since that information would come from outside the domain (See 3.2). The formulation of Zou and He conditions is based on a principle similar to the bounce back: the non-equilibrium part of the distribution functions whose directions are normal to the boundary must be equal (Zou and He, 1997).

To clarify this point take, for example, a velocity boundary on the left hand side of a 2D rectangular domain (figure 3.2a). According to the figure, the normal directions to the boundary are 1 and 5. So, the bouncing back of the non-equilibrium part of the distribution functions is described by the following expressions:

$$f_1^{in} - f_1^{eq} = f_5^{in} - f_5^{eq} \quad \Longrightarrow \quad f_1^{in} = f_5^{in} + f_1^{eq} - f_5^{eq} \tag{3.9}$$

The final form of the above expression is obtained by replacing the equilibrium distribution function 3.6, and it is shown in figure 3.3. The remaining unknown distribution functions, f_2 and f_8, are obtained by operating the f_1 expression with the macroscopic quantities equations, shown in 3.4. The equations for Zou and He velocity conditions for all four possible boundary positions are shown in figures 3.3 to 3.6. For pressure (density) conditions, just isolate the velocity component in the ρ expression.

3.2.2 Convective condition of the distribution functions

The convective condition of the distribution functions (f_i) was proposed by Yu et al. (2005). It consists in obtaining the unknown distributions functions of each outlet node copying it from a neighbor located in the opposite direction of the outlet, as shown in

$$
\begin{aligned}
\rho &= \frac{1}{1-u_x}[f_0^{in} + f_3^{in} + f_7^{in} + 2(f_4^{in} + f_5^{in} + f_6^{in})] \\
f_1^{in} &= f_5^{in} + \frac{2}{3}\rho u_x \\
f_2^{in} &= f_6^{in} - \frac{1}{2}(f_3^{in} - f_7^{in}) + \frac{1}{6}\rho u_x + \frac{1}{2}\rho u_y \\
f_8^{in} &= f_4^{in} + \frac{1}{2}(f_3^{in} - f_7^{in}) + \frac{1}{6}\rho u_x - \frac{1}{2}\rho u_y
\end{aligned}
$$

Figure 3.3: Zou and He equations for a left hand side wall.

$$
\begin{aligned}
\rho &= \frac{1}{1-u_y}[f_0^{in} + f_1^{in} + f_5^{in} + 2(f_6^{in} + f_7^{in} + f_8^{in})] \\
f_3^{in} &= f_7^{in} + \frac{2}{3}\rho u_y \\
f_2^{in} &= f_6^{in} - \frac{1}{2}(f_1^{in} - f_5^{in}) + \frac{1}{2}\rho u_x + \frac{1}{6}\rho u_y \\
f_4^{in} &= f_8^{in} + \frac{1}{2}(f_1^{in} - f_5^{in}) - \frac{1}{2}\rho u_x + \frac{1}{6}\rho u_y
\end{aligned}
$$

Figure 3.4: Zou and He equations for a bottom wall.

$$
\begin{aligned}
\rho &= \frac{1}{1+u_x}[f_0^{in} + f_3^{in} + f_7^{in} + 2(f_1^{in} + f_2^{in} + f_8^{in})] \\
f_5^{in} &= f_1^{in} - \frac{2}{3}\rho u_x \\
f_6^{in} &= f_2^{in} + \frac{1}{2}(f_3^{in} - f_7^{in}) - \frac{1}{6}\rho u_x - \frac{1}{2}\rho u_y \\
f_4^{in} &= f_8^{in} - \frac{1}{2}(f_3^{in} - f_7^{in}) - \frac{1}{6}\rho u_x + \frac{1}{2}\rho u_y
\end{aligned}
$$

Figure 3.5: Zou and He equations for a right hand side wall.

$$\rho = \frac{1}{1+u_y}[f_0^{in} + f_1^{in} + f_5^{in} + 2(f_2^{in} + f_3^{in} + f_4^{in})] \tag{3.10}$$

$$f_7^{in} = f_3^{in} - \frac{2}{3}\rho u_y \tag{3.11}$$

$$f_6^{in} = f_2^{in} + \frac{1}{2}(f_1^{in} - f_5^{in}) - \frac{1}{2}\rho u_x - \frac{1}{6}\rho u_y \tag{3.12}$$

$$f_8^{in} = f_4^{in} - \frac{1}{2}(f_1^{in} - f_5^{in}) + \frac{1}{2}\rho u_x - \frac{1}{6}\rho u_y \tag{3.13}$$

Figure 3.6: Zou and He equations for a top wall.

equation 3.14.

$$f_i^{in}(\boldsymbol{x}, t+\Delta t) = f_i^{in}(\boldsymbol{x} - \boldsymbol{e}_i\Delta t, t) \tag{3.14}$$

3.2.3 Convective condition of velocity

A recent proposal to deal with pressure wave reflection is the convective condition, by Yang (2013). The author compares it to other non-reflective conditions, such as the Do-nothing condition, the modified extrapolation method and the Grad's approximation. The comparison was made by transient simulations of flow around a circular and a square cylinder, paying special attention to the outflow influence to the overall fluid domain behavior, and the possibility of vortex destruction at the outflow boundary.

The convective velocity —condition for LBM, as well as similar boundary conditions proposed for other CFD methods, is intended to nullify the outflow strain rate ($S_{ij} = (u_{i,j} + u_{j,i})/2 = 0$), and is macroscopically equivalent to the expression in 3.15. The equations needed to apply the condition to LBM are shown in 3.16 and 3.17 (Yang).

$$\frac{\partial \boldsymbol{u}}{\partial t} + \bar{u}\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{n}} = 0 \qquad \begin{array}{ll} \boldsymbol{n} & \text{External normal at the outlet.} \\ \bar{u} & \text{Convective velocity.} \end{array} \tag{3.15}$$

$$\Delta \boldsymbol{u}_0 = -\frac{\bar{u}}{2}[3\boldsymbol{u}(\boldsymbol{x}, t) - 4\boldsymbol{u}(\boldsymbol{x} - \boldsymbol{n}, t) + \boldsymbol{u}(\boldsymbol{x} - 2\boldsymbol{n}, t)] \tag{3.16}$$

$$f_i^{in}(\boldsymbol{x}, t+1) = f_i^{out}(\boldsymbol{x}, t) + 3f_i^{eq}(\Delta \boldsymbol{u}_0 \cdot \boldsymbol{c}_i) \tag{3.17}$$

According to the author, the so called convective velocity must be positive and greater than zero, and suggest taking the average of the normal outflow velocity as a reasonable value. However, inspecting the physical quantities involved in equations 3.16 and 3.17 suggests that the convective velocity $\bar{u}$ is a dimensionless proportionality constant, not a velocity.

3.3 Fluid-Structure Interaction

This work makes use of the BFL boundary condition for the interaction of the fluid particles with a curved and movable boundary that does not fit into the lattice. Its name stands for the surnames of its authors: Bouzidi, Firdaouss, and Lallemand (2001). This boundary condition is based on the bounce back condition and spatial interpolations of the boundary position. The following equations were adapted from Caiazzo (2007).

$$\begin{aligned} f_i^{in}(\boldsymbol{x}, t+\Delta t) &= A(q) f_{i^*}^{out}(\boldsymbol{x}, t) \\ &+ B(q) f_{i^*}^{out}(\boldsymbol{x}+\boldsymbol{e}_i \Delta t, t) \\ &+ C(q) f_i^{out}(\boldsymbol{x}, t) \\ &+ 2D(q) t_i c_s^{-2} h\, \boldsymbol{u}_B \cdot \boldsymbol{e}_i \end{aligned} \tag{3.18}$$

$$A(q) = \begin{cases} 2q & q < 1/2 \\ \frac{1}{2q} & q \geq 1/2 \end{cases} \quad B(q) = \begin{cases} 1-2q & q < 1/2 \\ 0 & q \geq 1/2 \end{cases}$$

$$C(q) = \begin{cases} 0 & q < 1/2 \\ \frac{2q-1}{q} & q \geq 1/2 \end{cases} \quad D(q) = \begin{cases} 1 & q < 1/2 \\ \frac{1}{2q} & q \geq 1/2 \end{cases}$$

Where i^* is a lattice direction pointing to the solid and i is the opposite direction. q is the distance to the solid boundary, expressed as a fraction of the lattice link size. The constants A, B, C and D are function of the q distance. The momentum of the moving solid is transfered to the fluid by the term $\boldsymbol{u}_B$, which is the velocity of the solid. A scheme of this boundary condition is shown in figure 3.7 for $i = 5$.

(a) Right side of the equation (b) Result. Left side of the equation

Figure 3.7: Example scheme of applying the BFL boundary condition for $i = 5$

According to Caiazzo (2007), the initialization of new fluid nodes that appear while the solid is moving can be done assigning equilibrium distribution function and information from surrounding nodes, which is called equilibrium plus non-equilibrium refill. This approach led to pressure inconsistencies around the moving boundary. The best possible results were met using a full non-equilibrium refill, i.e, extrapolating the distribution functions of the surrounding nodes to each new fluid node.

Although there are lattice Boltzmann based procedures to compute the strain rate tensor over curved and mobile boundaries, a more traditional CFD procedure was used:

- The lattice is treated as a fixed grid, considering cells formed by four lattice nodes.
- Then, cells can be classified in three categories: inside solid, outside solid, and NIO (nor inside or outside).
- The NIO elements, which contain the curved boundary, are completely identified.
- Each NIO can contain from one to three special fluid nodes, which are the nearest fluid nodes to the curved boundary. These are called curved nodes.
- The average pressure p of each NIO can be computed from the pressure of its curved nodes.
- From each NIO, a triangle of the best aspect ratio is formed using a curved node and the boundary section that crosses the NIO cell. This triangle is used to compute the velocity gradient, taking into account velocities from fluid and solid domains.

- The strain rate tensor D of each NIO cell can be easily computed from the velocity gradient.
- The normal $\boldsymbol{n}$ and the length L of each boundary section contained inside a NIO has to be measured in order to compute the distributed force over that section.

Having computed the aforementioned values, the total stress tensor σ and the distributed force $\boldsymbol{F}$ of each NIO can be easily obtained using the following equations.

$$\sigma = 2\mu D - pI \tag{3.19}$$

$$\boldsymbol{F} = (\sigma \cdot \boldsymbol{n})L \tag{3.20}$$

Finally, force information computed using lattice Boltzmann method can be transferred to a solid domain resolution method, as discussed in section 2.2 about partitioned approaches of fluid-structure interaction. Then, the structural solver is responsible for obtaining the displacements and deformations, and returning the modified geometry and the momentum to the fluid. This process is repeated each time step until an adequate solution to the problem is found.

Chapter 4

Numerical tests

The present chapter contains various numerical tests of the lattice Boltzmann method, which were performed in order to show that it can be used for fluid-structure interaction, even using its simplest formulation: the lattice Boltzmann method with single relaxation time (LBM-BGK). However, the results also show that there are still good possibilities of developing better boundary conditions for transient problems, not only limited to outlet boundaries.

Studies on analysis and development of open boundary conditions have focused primarily on vortex shedding benchmarks, where the outflow boundary conditions are studied in order to determine whether they are pressure wave reflective or not (see, for example, Izquierdo et al., 2009, and Yang, 2013). However, in such simple cases as laminar Poiseuille flow the oscillations are also present, even tough there is no visible source for them.

The numerical tests are performed using an in-house C++ code, which uses a standard LB-BGK model and a D2Q9 lattice. The showcases studied are the Poiseuille flow and the circular cylinder benchmark, and the results are expressed in physical units for comparison with commercial CFD software results (ANSYS CFX for this case).

With exception of the solid obstacle or the lattice resolution, all tests share the same parameters: each simulation consists of an unsteady flow of glycerol, traveling from left to right through a 2D closed channel with a Reynolds number of 20 and a temperature of 20°C ($\rho_r = 1263.97$ kg/m^3, $\mu_r = 1.48913$ kg/(m s)). The bounce back condition is applied to the top and bottom walls of the channel to simulate no-slip, and unless otherwise stated, a Zou and He velocity boundary condition is used for inflow. The dimensions of the domain

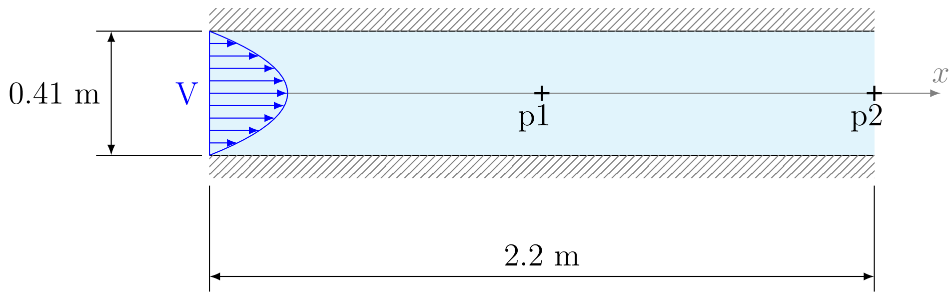


Figure 4.1: Scheme of the domain for simulations of fluid flow without obstacles.

are shown in figure 4.1.

To avoid other sources of oscillations, like compressible effects, the diffusive scaling is applied for all the simulations. Furthermore, an effort for reducing the inconsistency of initial conditions is done by including an initialization stage: inlet velocity is increased steadily from zero to the maximum velocity defined by the Reynolds number. No additional considerations are taken regarding initial layers.

The minimum duration of the initialization stage is defined as the amount of time taken by a particle to travel through the entire domain. For Poiseuille cases, the initialization stage was set to 88.84 seconds, and for the circular cylinder cases the initialization time was set to 18.67 seconds.

The simulations contained in this chapter are:

- Comparison of the influence of the outlet boundary conditions on the stability of the domain, using a probe located at the middle point P1 (fig 4.1). This is done using Poiseuille flow and the analyzed variables are pressure and horizontal velocity.

- Comparison of mass conservation for various outlet boundary conditions. The horizontal velocity is measured along the X axis when the Poiseuille flow simulations have reached the steady stage and the oscillations have ceased.

- An exploration of the convective boundary condition, to determine an appropriate value for the convective velocity $\bar{u}$. This is done using the Poiseuille flow. Then, tests of stability and mass conservation are repeated with the best convective velocity.

- Computation of the drag coefficient, using flow around a circular cylinder. The validation of the result is made by a lattice sensitivity analysis of the drag coefficient and comparing with reported values.

- Influence of a moving curved boundary in a quiescent fluid. This is done in order to verify whether this movement produces oscillations, and its dependence on the lattice resolution. Convective conditions of the distribution functions (Yu et al., 2005) are used for all four edges of the fluid domain.

- Ignoring wall condition. This simulations shows that a big cause of fluid disturbance and pressure wave generation may be the bounce back boundary condition.

4.1 Influence of the outlet conditions in the domain stability

The objective of this test is to verify if the compared boundary conditions are reflective, and how much they affect the stability of the domain. This is done through the simulation of a Poiseuille flow, measuring the fluid behavior at the middle point P1 over time. The variables of interest are pressure and horizontal velocity.

The compared boundary conditions are the Zou and He velocity condition and the convective condition of the distribution functions. Convective condition of velocity will be compared in a subsequent test, due to the fact that a good value for the convective velocity remains unknown, and a exploration of this value will be developed first.

The results of lattice Boltzmann boundary conditions are compared to ANSYS CFX results. For this simulation, a structured mesh of 220×41×1 hexahedra was used, and as well as the lattice Boltzmann simulations, the inflow is steadily accelerated from zero.

The lattice resolution chosen for the test is 221×41 nodes, taking 41 spaces of height as the characteristic length ($N = 41$). The characteristic time, regarding diffusive scaling, is 1681 time steps ($N_t = 1681$). Results of this test are shown in figures 4.2 to 4.3.

Figure 4.2 shows the change of velocity over time at the middle point of the domain for each boundary condition. It can be observed that both kind of boundary conditions reach an steady state, and both present oscillations, although it is hardly noticeable for the case of convective f_i condition. Velocity differences regarding ANSYS results are expected, due to the fact that the chosen lattice resolution may not be enough refined. However, there should be no difference in the final velocity of both boundary conditions considered.

As stated before, except for the boundary condition type, the simulation parameters

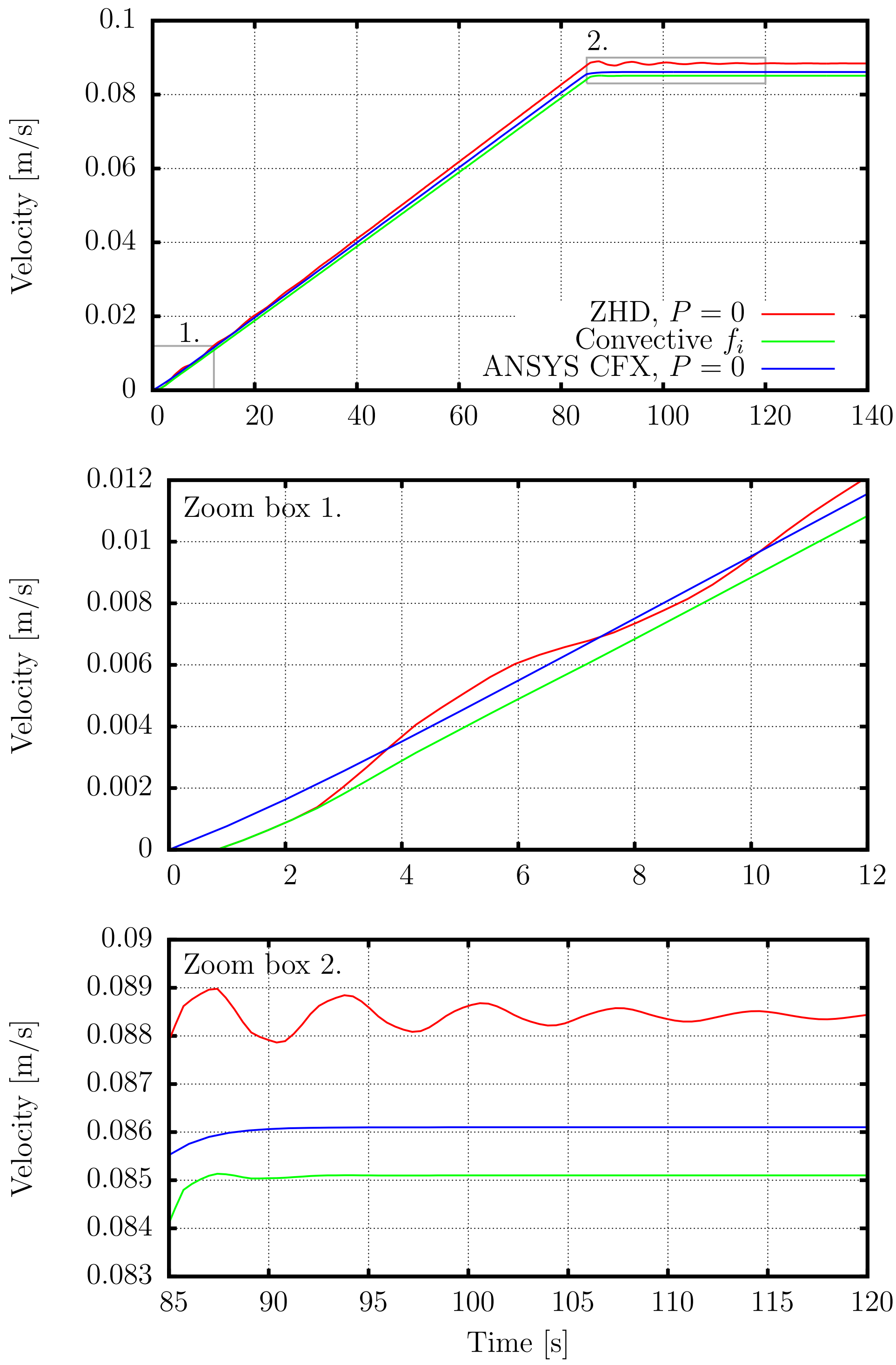


Figure 4.2: Opening boundaries comparison. Change of velocity over time at the middle point of the domain.

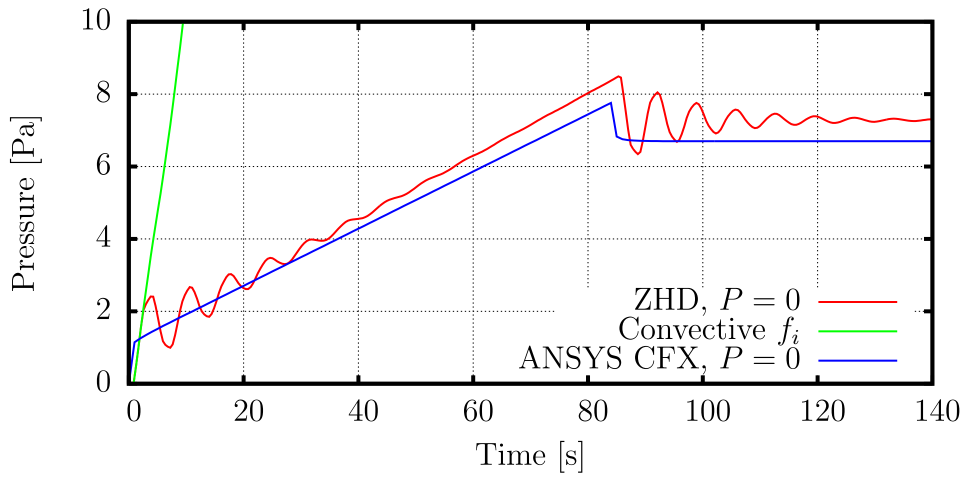


Figure 4.3: Opening boundaries comparison. Change of pressure over time at the middle point of the domain.

for both boundary conditions are identical. The velocity difference suggest a possible violation of the principle of mass conservation in one or even both cases. This situation will be verified in the next section.

Figure 4.3 shows the change of pressure over time for both conditions, measured in the middle point of the domain. The most striking detail that can be seen from this figure is the behavior of the convective condition: its pressure never stops growing, even if the inflow has a constant velocity. This would be a serious problem to compute the hydrostatic component of stress for a fluid-structure interaction problem.

As it can be seen in section 3.2.2, the convective condition of the distribution functions is a weaker restriction than Zou and He conditions: it only requires that the unknown distribution functions on the outlet boundary remain equal to the values near that boundary, while the macroscopic quantities (velocity and pressure) are unrestricted.

For the other case, the Zou and He density condition is the only one restricting the outlet pressure, and hence the inner pressure too. The other three boundaries, Zou and He velocity inlet and bounce back walls, are non-restrictive of the pressure. Results of this case actually exhibit a similar behavior to those obtained by ANSYS, although oscillations can be clearly observed.

The results obtained so far show that lattice Boltzmann method requires a pressure (or density) restriction in any of its boundaries in order to obtain acceptably good results

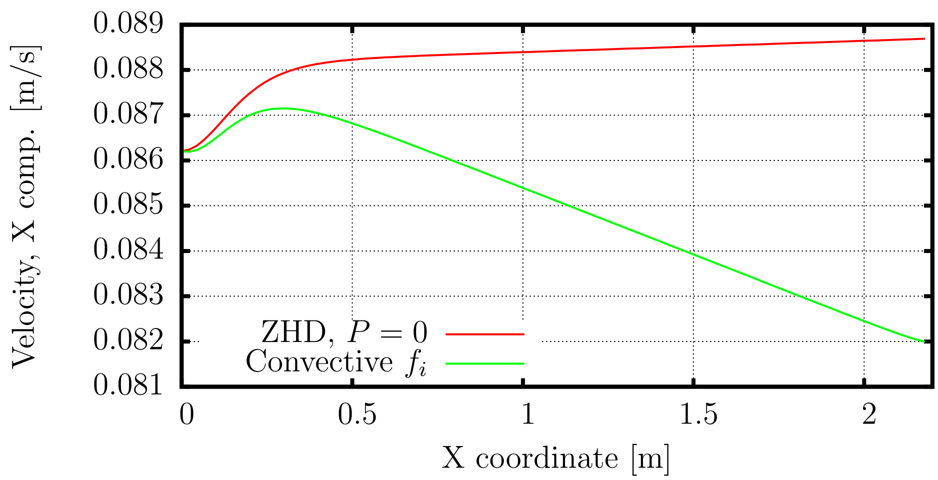


Figure 4.4: Opening boundaries comparison. Change of the X component of velocity along the X axis at steady state.

for both pressure and velocity in the steady state. The convective f_i case, having no pressure boundary restriction, allows the inner pressure to grow indefinitely.

4.2 Influence of outlet boundaries on the mass conservation compliance

For this test, the results of the Poiseuille flow of the previous test are revisited. The objective is to verify whether the simulations of each boundary conditions comply the mass conservation principle when they reach the steady state. The verification can be easily accomplished by measuring the horizontal velocity along the X axis and checking whether its function is constant or not. The results for this test are shown in figure 4.4.

It can be seen that both conditions fail the mass conservation principle, although this is more critical for the convective f_i condition. It can be also seen from figure 4.4 that there is a curvature change in the left hand side of both curves. This may suggest that the inlet boundary condition is leading a strange behaviour of its surroundings.

4.3 Exploration of the convective condition of velocity

As noted previously, the convective velocity $\bar{u}$ is an scalar quantity required by the convective condition formulation, for which there is not enough information nor criteria to assign it a value. It is suspected that this variable is not a velocity but a proportionality constant. This test is intended to explore some values of the convective velocity to find, if possible, an appropriate one.

Apart from the outlet condition, this test will be identical to earlier tests: first, physical velocity and physical pressure are measured over time to determine the best convective velocity. Then, the convective velocity condition is compared with Zou and He conditions for both velocity and pressure over time. Finally, mass conservation test is repeated for convective velocity condition.

The range of appropriate values for the convective velocity is limited by the stability of the simulation. It was verified that negative values are not valid, but was not possible to obtain stable simulations beyond a value of 0.55. Results for this test are shown in figures 4.5 to 4.9.

Figure 4.5 shows the velocity change rate at the middle point for 5 different values of convective velocity. It can be noted that the convective velocity condition shows a similar pattern of velocity oscillations regarding Zou and He conditions, even at the beginning of the simulations. Beyond $\bar{u} = 0.01$ the results improvement is hardly noticeable. The best velocity results improvement were obtained using $\bar{u} = 0.55$.

The pressure results for convective velocity condition are similar to those obtained for velocity (figure 4.6): they exhibit a similar pattern of oscillations when compared to Zou and He velocity condition results, and their best results are obtained again using $\bar{u} = 0.55$. However, oscillations reduction does not seem very significant compared to the overall results.

When the velocity change rate results of the convective condition is compared with Zou and He condition, it can be seen a very little reduction of the oscillations (fig. 4.7). Regarding pressure results, there is not a clear reduction of the oscillations, although the pressure inside the domain does not diverge, such as the case of convective f_i condition (fig. 4.8).

Figure 4.9 shows that, as well as the other boundary conditions presented here, convec-

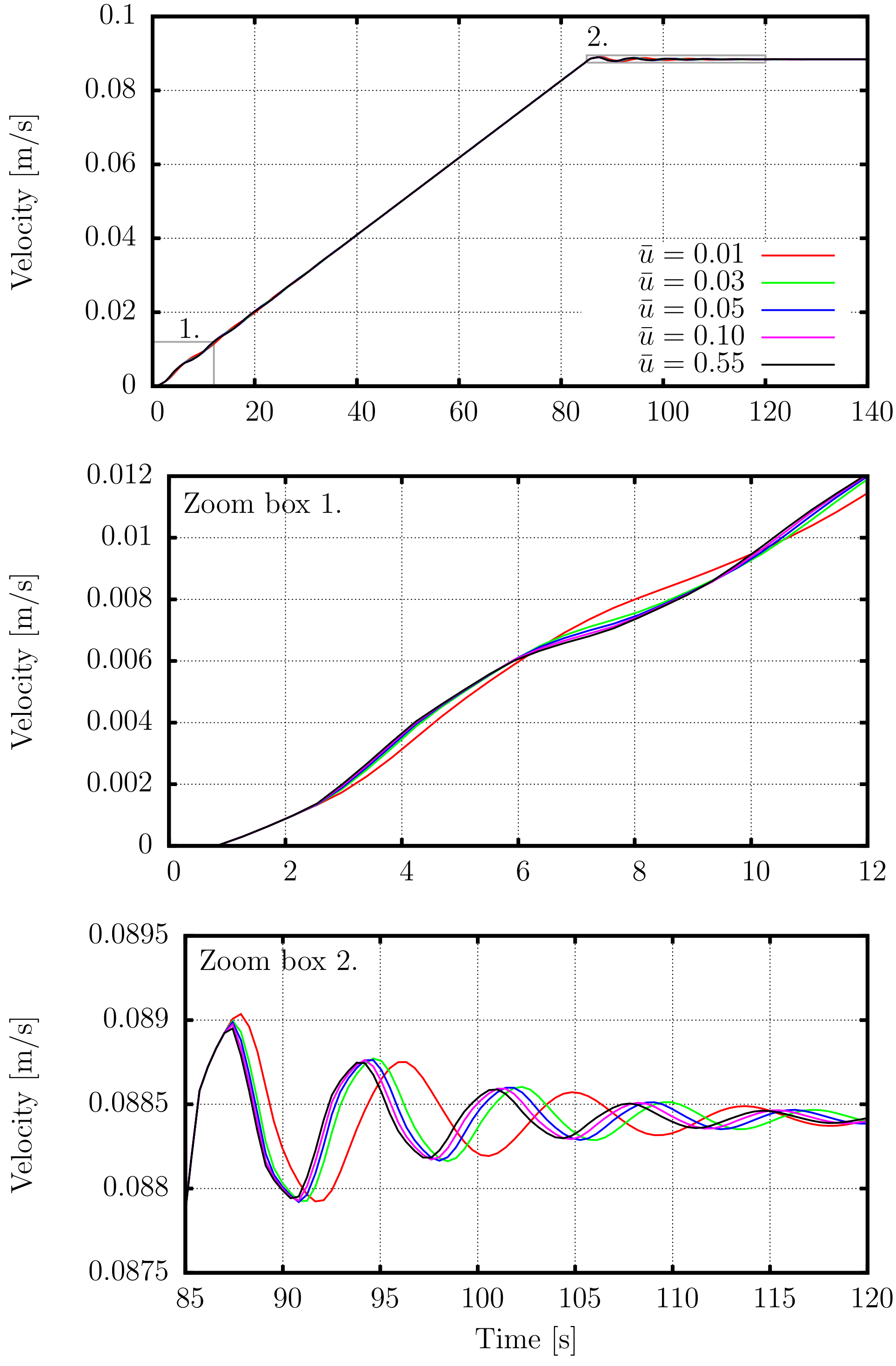


Figure 4.5: Convective velocity condition. Change of velocity over time at the middle point of the domain.

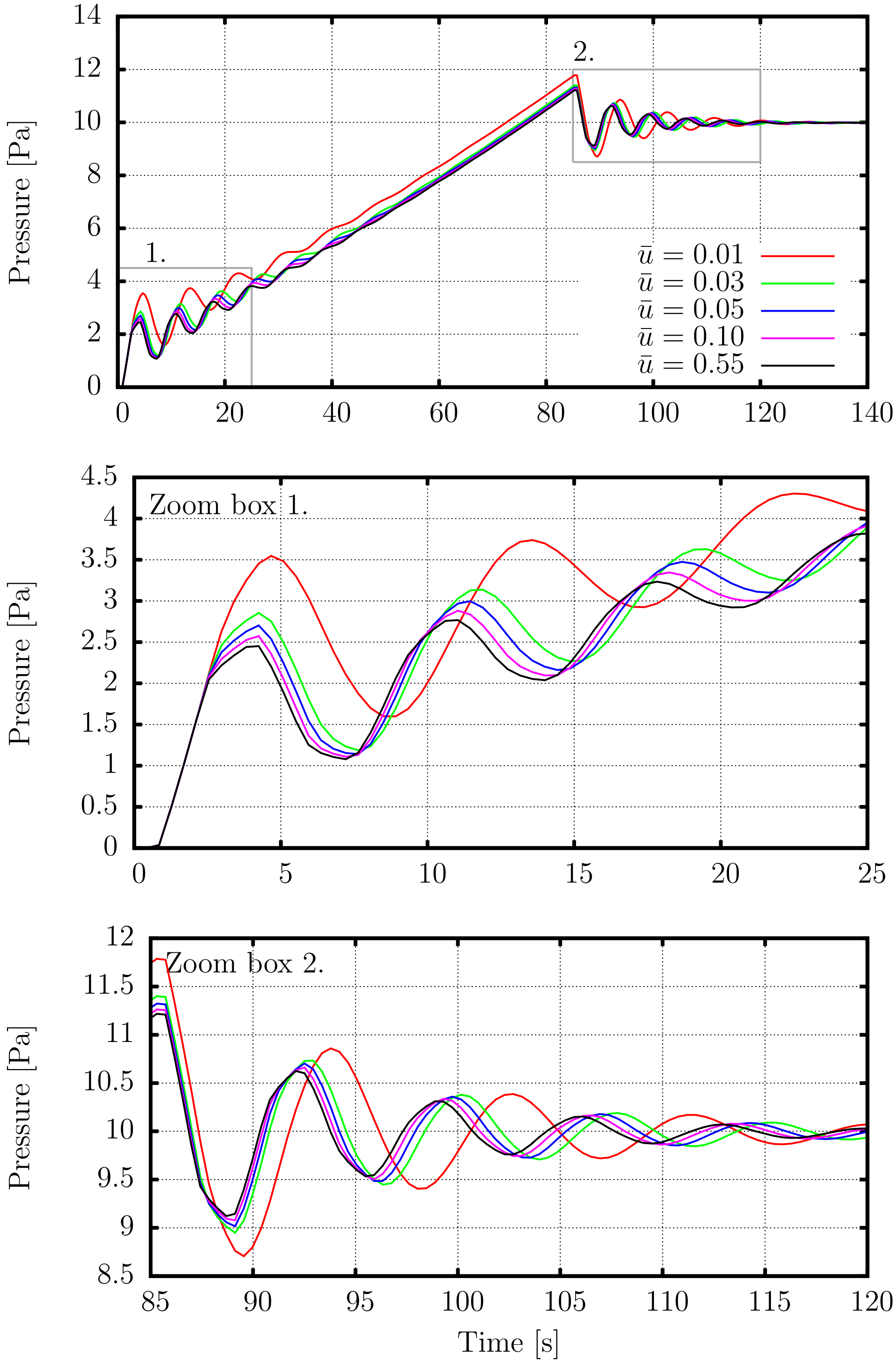


Figure 4.6: Convective velocity condition. Change of pressure over time at the middle point of the domain.

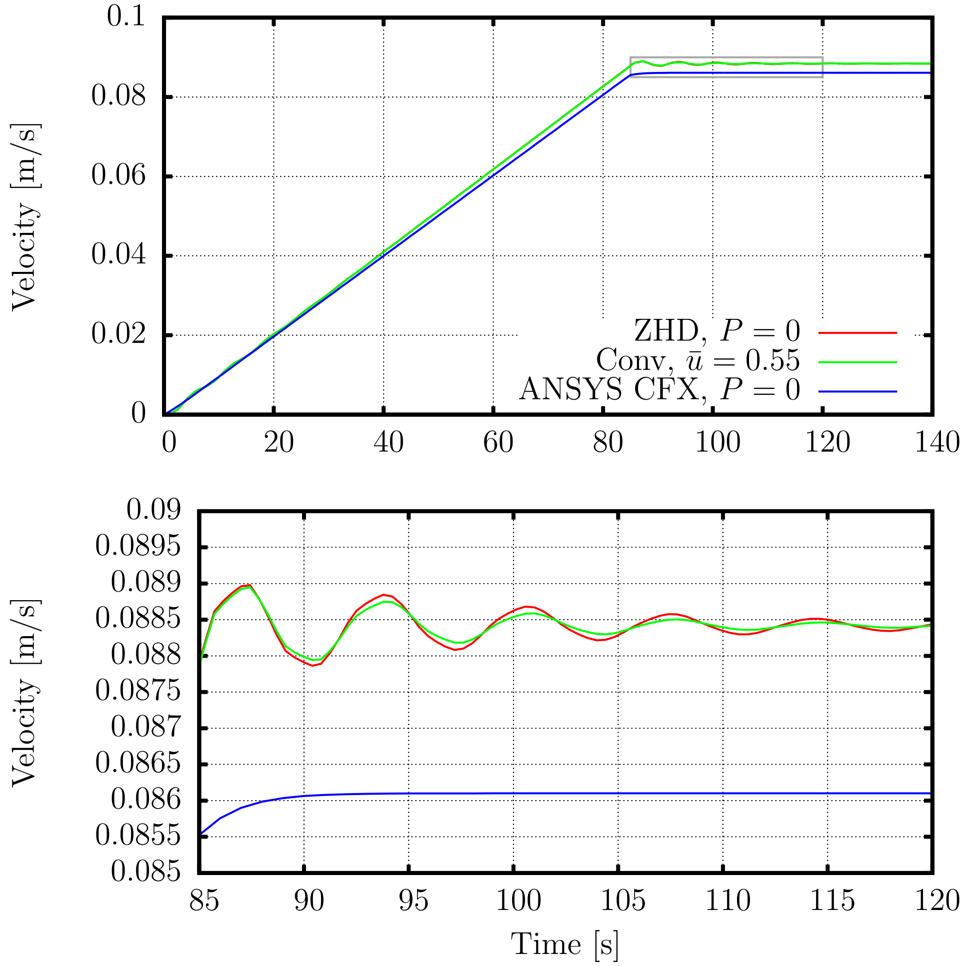


Figure 4.7: Convective velocity vs others. Change of velocity over time at the middle point of the domain.

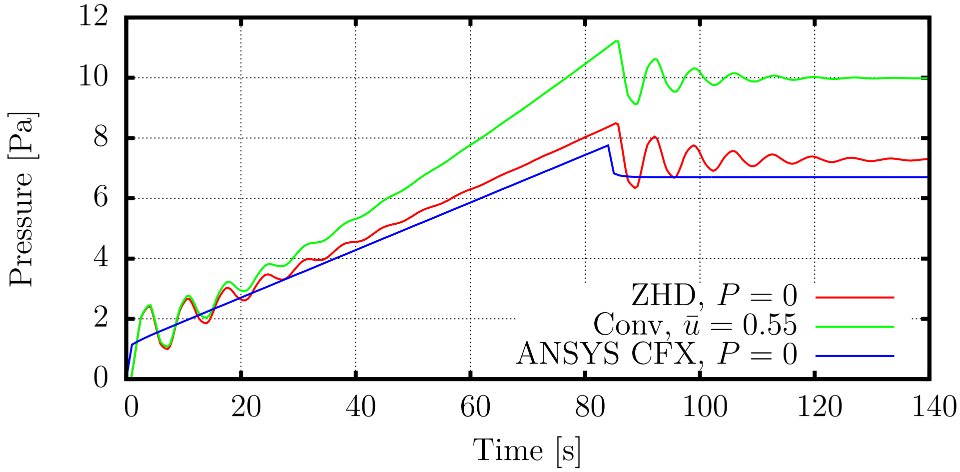


Figure 4.8: Convective velocity vs others. Change of pressure over time at the middle point of the domain.

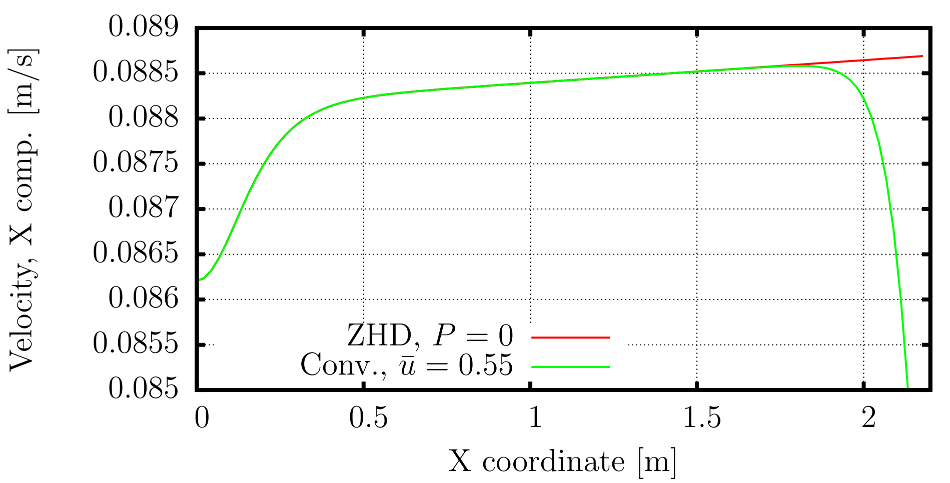


Figure 4.9: Convective velocity vs others. Change of the X component of velocity along the X axis at steady state.

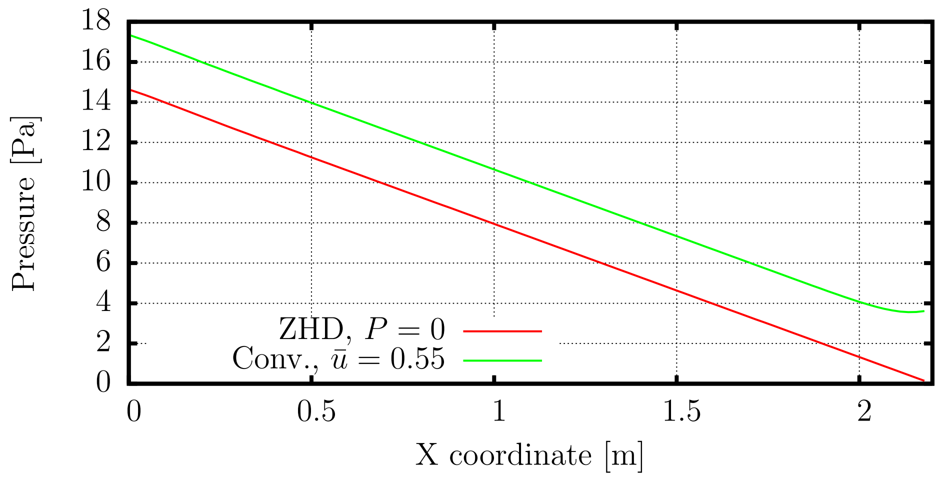


Figure 4.10: Convective velocity vs others. Change of pressure along the X axis at steady state.

tive condition of velocity does not comply with the mass conservation principle. It shows a very similar behavior to the Zou and He velocity condition, except near the outlet, where convective velocity case presents an steep decrease of velocity.

Checking also the pressure gradient along the X axis (figure 4.10), both conditions show very similar behavior, but the exception at the outlet appears again. The convective velocity case shows a greater pressure than the Zou and He velocity case, but it also seems to stop near the outlet, where its pressure gradient disappears.

A fact that is well known from fluid dynamics fundamentals is that a pipe flow does not occur unless a pressure gradient exists. Thus, the absence of pressure gradient near the outlet of the convective velocity case can explain the velocity drop in this zone. The convective velocity condition, at least at the particular value chosen at 0.55, seems to be over-restrictive for the simulation.

4.4 Drag coefficient of a circular cylinder

The purpose of this test is to verify the ability of the method, in conjunction with the BFL boundary condition, to calculate the forces on a curved boundary. The benchmark used for this test is the flow around a circular cylinder, using a 10 cm diameter cylinder and the same domain and parameters used for above tests. A lattice sensitivity analysis

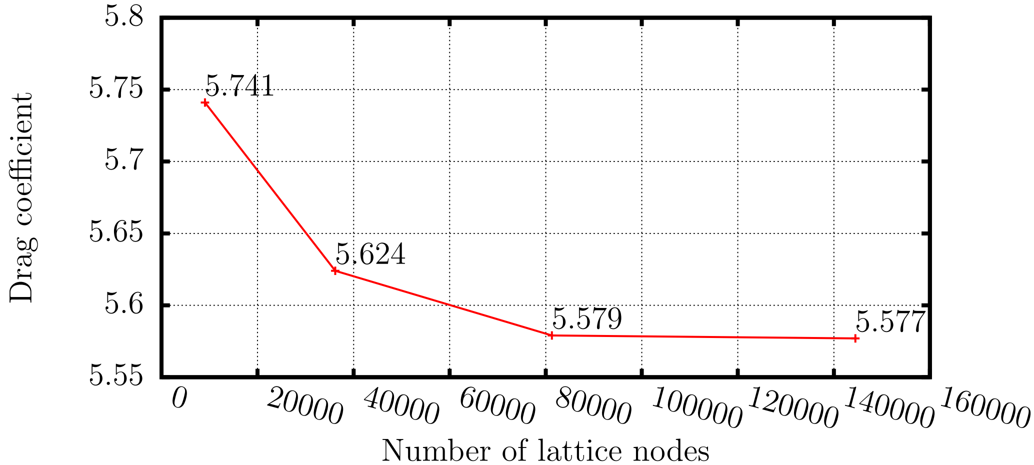


Figure 4.11: Drag coefficient. Lattice sensitivity analysis of the circular cylinder benchmark.

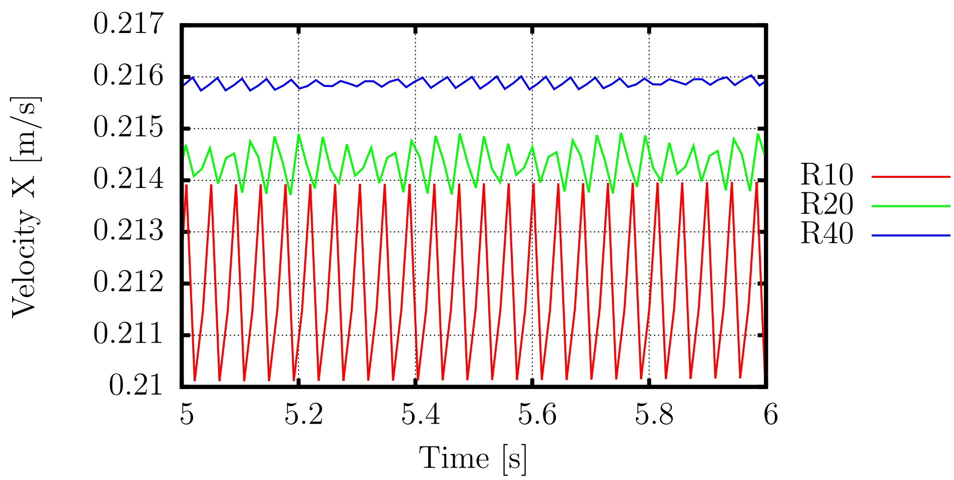
is carried out, in order to compare the drag coefficient with the values obtained in the report of Schäfer et al. (1996).

Results of the sensitivity analysis are shown in figure 4.11. The drag coefficient value of 5.577 shows good agreement with results obtained by Schäfer et al. (1996).

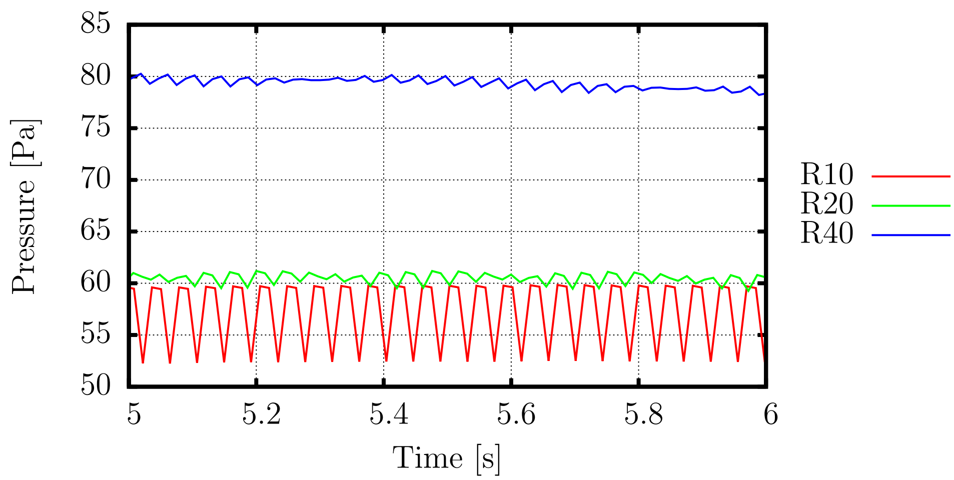
4.5 Influence of a moving cylinder in a quiescent fluid

This test consist in measuring the macroscopic variables in the surroundings of the moving solid boundary, seeking possible perturbations related with lattice resolution. To accomplish this, the cylinder moves with a constant velocity of 0.2356 m/s (Re = 20) through the domain, while a moving prove located 1 cm in front of the cylinder measures pressure and velocity. Convective f_i condition is applied on the four edges of the fluid domain to avoid spurious bouncing pressure waves.

It can be observed from figure 4.12 that the moving cylinder produces oscillations while it moves through the fluid domain. Despite the fact that they suffer an important reduction from the first lattice refinement (doubling resolution from 10 to 20 lattice units of diameter), the reduction, if any, is not quite observable when the lattice resolution is doubled again. However, it is also noticeable that perturbations caused by the curved moving boundary are not as severe as the straight boundary effects.



(a) Velocity



(b) Pressure

Figure 4.12: Macroscopic variables near cylinder. Comparison for various lattice sizes

4.6 Ignoring boundary conditions at the walls

The aim of this test is to show what happens when the streaming of information to a wall is turned off completely. To do this, a Poiseuille flow simulation is performed, using conventional Zou and He conditions on both ends of the channel, i.e, inlet velocity and outlet pressure, while walls are "ignored". The procedures of the first and second test are repeated for this one: the presence of oscillations and the mass conservation are verified. It is worth mentioning that ignoring wall approach should not be confused with do-nothing condition, which was proposed by Junk and Yang (2008).

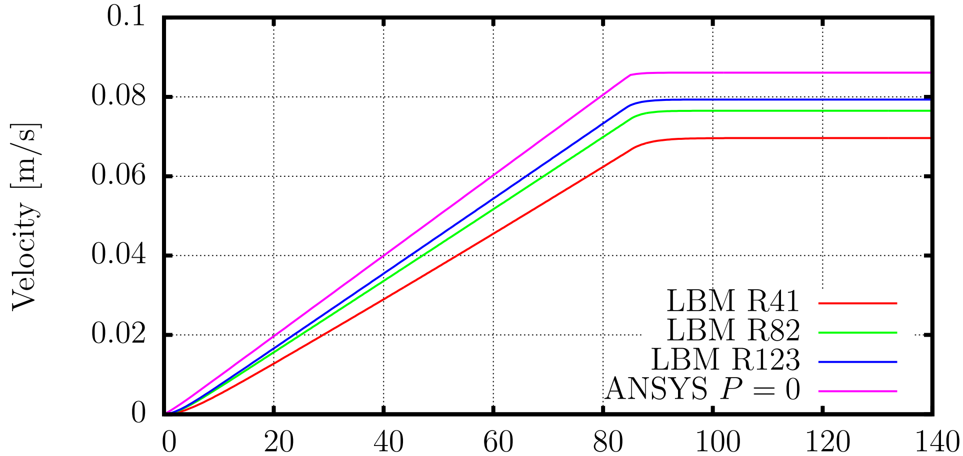
As it could be seen in section 3.1, streaming step is an essential procedure of the lattice Boltzmann method, since it allows to update mass and momentum information of the distribution functions of each node. When this update is not allowed to happen towards wall nodes, their incoming distribution functions remain constant. Accordingly, outgoing distribution functions are not updated either, since collision step depends exclusively on incoming information. Finally, near wall nodes renew its information from inner nodes only, due to the fact that information that came from the walls is constant.

Results are shown in figures 4.13 and 4.14. Figure 4.13a shows the variation of velocity over time at the middle point of the domain. It can be noticed that velocity remains stable for all the evaluated resolutions, and they also look similar to ANSYS results. Similar observations can be done for figure 4.13b, where the pressure function looks very similar for all LBM and ANSYS results, with no sightable oscillations.

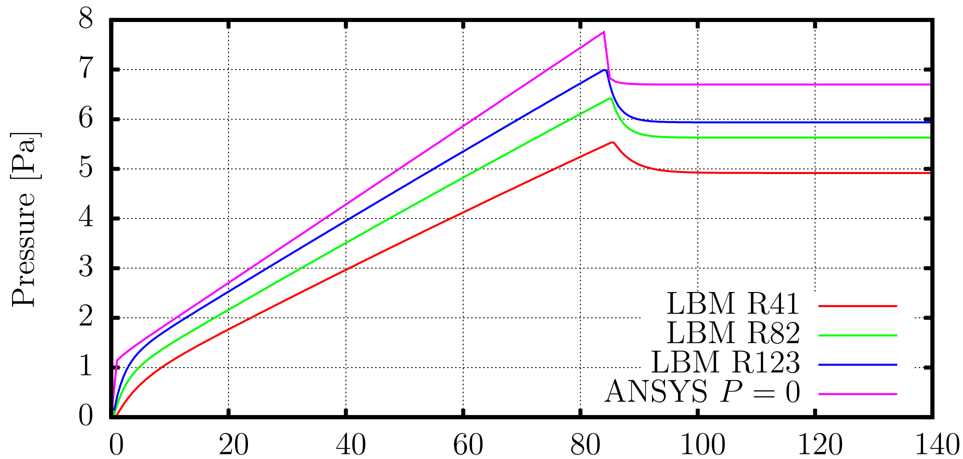
Both figures show that is possible to obtain a more approximated result to ANSYS by refining the lattice resolution, or maybe using a local refining near the walls, to avoid excesive computational effort for the rest of the domain. However, this approach is not considered as a new boundary condition, but a simple practical demonstration that the bounce back boundary condition may be the biggest cause of spurious pressure wave generation of LBM fluid flow problems.

Figure 4.14 shows the variation of horizontal velocity along the X axis of the domain. It shows that, as well as other boundary conditions tested in this work, ignoring wall conditions does not comply with the mass conservation principle, although refining the lattice would improve this result. Failure in mass conservation principle would be a good reason to develop a better non-slip boundary condition.

The results of this last test show also that the lattice Boltzmann equation, which



(a) Velocity



(b) Pressure

Figure 4.13: Ignoring wall conditions. Variation of macroscopical variables at the middle point over time for various lattice resolutions

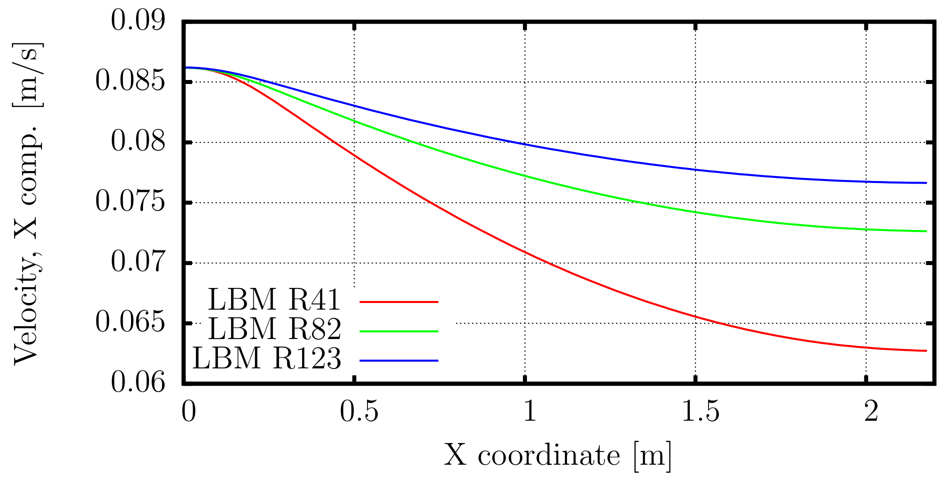


Figure 4.14: Ignoring wall conditions. Change of the X component of velocity along the X axis at steady state, for various lattice resolutions

governs all the inner fluid nodes that are away from boundaries, is an excellent tool for simulating incompressible fluid flow problems, as demonstrated by several (theoretical) papers on asymptotic analysis, and this efficiency to describe the fluid behavior is inherited from statistical mechanics. A more physical approach, not bouncing, may be required to develop an appropriate non-slip boundary condition for unsteady problems.

Chapter 5

Conclusions

- Lattice Boltzmann method appears as a good alternative to traditional CFD methods for solving steady fluid flow problems. However, pressure waves appear while trying to obtain solutions of unsteady problems, even when some measures to avoid them are taken, like diffusive scaling, or initializing the fluid by increasing steadily its inlet velocity.

- Velocity oscillations were observed for all the outlet boundary conditions studied in this work, although they were hardly noticeable in the case of the convective condition of the distribution function. However, this boundary condition causes a steadily growth of the pressure inside the domain, making impossible to compute the hydrostatic component of stress for a fluid-structure interaction problem.

- The whole set of outlet boundary conditions studied in this work exhibits failures to comply the principle of mass conservation. This suggest that the method may require improvements in other aspects besides the outlet conditions. For example: alternatives to the bounce back condition for no-slip wall.

- The convective boundary condition studied for this work is very simple to implement. However, no significant improvement was observed with respect to the Zou and He density condition for the Poiseuille flow test problem. Both of them show pressure oscillations, which are not considered a problem for steady cases, but they definitely cause non negligible errors in the calculation of hydrostatic forces for unsteady problems.

- Initialization strategies may be required to set initial values to the distribution functions, given that pressure oscillations appears at the beginning of the simulations and even when the velocity is increased steadily from zero.

- New and non-oscillating results were obtained by switching off the streaming step of the non-slip boundaries, typically simulated using bounce back conditions. This approach shows that it is possible to obtain better unsteady results than more conventional LBM approaches outlined here, being even comparable to those obtained through commercial finite volume CFD software, although these do not comply with the mass conservation principle.

- It is proposed as future work: *i* a rigorous analysis of the physical and mathematical implications of ignoring the boundary, and *ii* a non-slip boundary condition, suitable for unsteady flows, and compliant of the mass conservation principle.

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