12º CONGRESSO BRASILEIRO DE PESQUISA E DESENVOLVIMENTO EM PETRÓLEO E GÁS

TÍTULO DO TRABALHO:

High Reynolds number flow simulation in a square duct using the lattice Boltzmann method.

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Abstract:

We present a new approach to modeling the flow in a square using the lattice Boltzmann method in an environment with wall constraints through boundary conditions for a turbulent case. The method employs a regularized version of the lattice Boltzmann equation. The reconstruction of regularized particle populations is based on second-order moments of the distribution function. Based on the work of Hegele Jr et al. (2018), our approach reconstructs unknown moments by means of known particle populations at the boundary, leading to a system of linear equations, solved before the simulations. Thus, the proposed approach increases accuracy and stability at high viscosities without compromising performance and amenability to parallelization with respect to standard lattice Boltzmann models. The three-dimensional stencil D3Q19 is considered for the solution of a square duct as a reference test. Comparison with literature solutions shows excellent agreement, validating the effectiveness of the proposed method.

Keywords: Square duct, Lattice Boltzmann method, Numerical simulation.

1. INTRODUCTION

The study of fluid flow in complex geometries is of fundamental importance in various fields of engineering and applied sciences (Lee, You-Hsun, 2018). Square ducts, in particular, are frequently encountered in ventilation systems, heat exchangers, and numerous industrial processes. A detailed understanding of the flow behavior within these ducts can lead to significant improvements in the efficiency and performance of these systems. Traditionally, the analysis of flow in ducts has been performed using computational fluid dynamics (CFD) methods based on the Navier-Stokes equations. However, these approaches can be computationally intensive and complex, especially when dealing with unconventional geometries and complicated boundary conditions. (White, 2006) The Lattice Boltzmann Method (LBM) emerges as a promising alternative due to computational efficiency. Unlike conventional methods based on partial differential equations, the LBM is founded on modeling the dynamics of the fluid's constituent particles using a discrete grid in space and time. This approach allows for a simpler and more flexible implementation for simulating flows in arbitrary geometries. In this work, we investigate the flow of a fluid within a square cross-section duct using the Lattice Boltzmann Method. We explore flow characteristics such as velocity and pressure profiles and compare the obtained results with analytical solutions and experimental data available in the literature. Additionally, we analyze the computational efficiency of the method and discuss its advantages and limitations in the context of a square duct flow.

2. METHODOLOGY

2.1 LATTICE BOLTZMANN METHOD

The lattice Boltzmann method involves solving the Boltzmann equation for the hydrodynamic behavior of fluids discretely in velocity and time space using numerical methods. The LBM method is considered to be a mesoscopic model for simulating the behavior of fluids, with the ordering and interactions of the particles being through a discrete network. The distribution function f_i is used to represent the macroscopic properties of a fluid, such as density, as well as the velocity vector of the unit particle ci at each time step at its respective site. The method consists of initially defining a distribution function for the model domain and successively colliding and propagating the particles, reordering the chain at each time step, this process is called the evolution of the distribution function as can be seen in Eq.5 (Kruger, 2016):

$$f_i(x + c_i, t + 1) = f_i^{(eq)}(x,t) + (1 - \tau^{-1})\hat{f}_i^{(neq)}(x,t), \tag{1}$$

$$\nu = c_s^2 \left(\tau - \frac{1}{2}\right)\Delta t, \tag{2}$$

where $f_i^{(eq)}$ and $\hat{f}_i^{(neq)}$ are the equilibrium and regularized non-equilibrium particle distribution functions, while x, c_i, and t represent space, microscopic velocity, and time, respectively, in dimensionless units and the relaxation time τ controls the relaxation of the viscous stress in the fluid and is linked to the kinematic viscosity ν present in Eq.6 (Hegele Jr. et al.,2018).

The Hermite polynomials of 0th, 1st and 2nd order were introduced into the particle distribution equation with the initial polynomials where δαβ represents the Kronecker delta, and as = √3 serves as a scaling factor.

$$H_i^{(0)} = 1, \tag{3}$$

$$H_{\alpha,i}^{(1)} = c_{i\alpha}, \tag{4}$$

$$H_{\alpha\beta,i}^{(2)} = c_{i\alpha}c_{i\beta} - \frac{\delta_{\alpha\beta}}{a_s^2}, \tag{5}$$

The regularized distribution function is adjusted every timestep and takes into account density ρ, the 0th-order moment, the momentum ρu, the 1st-order moment, and the moments ρm(2) αβ , the 2nd-order moments for updating the whole domain Succi (2001); Hegele Jr. et al. (2018):

$$\rho = \textstyle\sum_i f_i, \tag{6}$$

$$\rho u_\alpha = \textstyle\sum_i f_i c_{i\alpha}, \tag{7}$$

$$\rho m_{\alpha\beta}^{(2)} = \textstyle\sum_i f_i H_{\alpha\beta,i}^{(2)}, \tag{8}$$

Introducing the second-order moments, we get:

$$\{\rho, \rho u_\alpha, \rho m_{\alpha\beta}{}^{(2)}\} = \sum_i g_i\{1, c_{i\alpha}, c_{i\alpha}c_{i\beta} - \delta_{\alpha\beta}/a_s{}^2\}, \tag{9}$$

Applying the Hermite polynomials to the equations of the distribution function and the regularized distribution function, we obtain the following Eq. 10 and Eq.11 (Montessori et al., 2024).

$$f_i^{(eq)}(\boldsymbol{x}, t) = \rho w_i \left(1 + a_s^2 u_\alpha c_{i\alpha} + \frac{1}{2} a_s^4 u_\alpha u_\beta H_{\alpha\beta,i}^{(2)}\right) \tag{10}$$

$$\hat{f}_i^{(neq)}(\boldsymbol{x}, t) = \frac{1}{2}\rho w_i a_s^4 \left(m_{\alpha\beta}^{(2)} - u_\alpha u_\beta\right) H_{\alpha\beta,i}^{(2)} \tag{11}$$

Our model uses a D3Q19 stencil in which the focal point interact with the other eighteen neighbors points in the system. Each point in the network is represented by a distribution function fi, which represents the speed and direction of each particle on a microscopic scale and the sum of this function represents the macroscopic properties of this flow (Kruger, 2016).

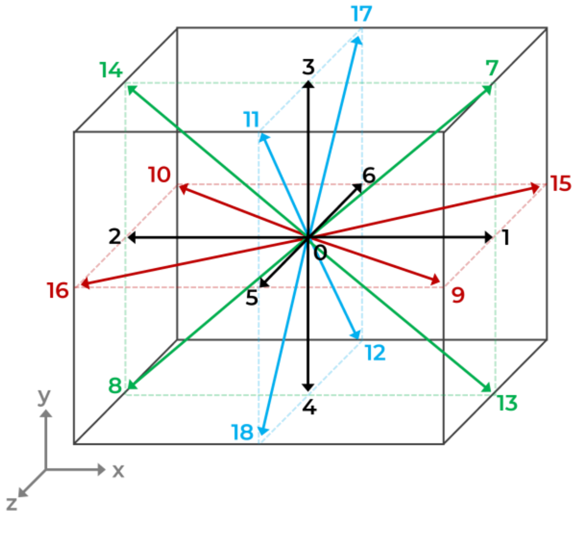

Figure 1. **Representation of D3Q19 model with the velocity vectors of the stencil poiting from the origin.**

Additional parameters are required where w_i refers to the weight values for each direction indicated and c_i corresponds to the velocity vectors directed towards neighboring sites.

$$w_i = \begin{cases} 1/3, & i = 0 \\ 1/18, & i = 1, \ldots, 6 \\ 1/36, & i = 7, \ldots., 18 \end{cases} \tag{12}$$

$$c_i = \begin{cases} (0,0,0), & i = 0 \\ (\pm 1,0,0),\ (0,\pm 1,0),\ (0,0,\pm 1), & i = 1, \dots, 6 \\ (\pm 1,\pm 1,0),\ (\pm 1,0,\pm 1),\ (0,\pm 1,\pm 1), & i = 7, \dots, 18 \end{cases} \tag{13}$$

2.2 BOUNDARY CONDITIONS

For the mesh domain of the visible rectangular volume, an [x, y, z] Cartesian grid of [128, 128, 768] was used with the West, East, Front and Back faces obeying the Dirichlet conditions and the North and South faces in periodic conditions Fig.2 The units used during method development and analysis of results are based on simulation time steps and domain lattice points.

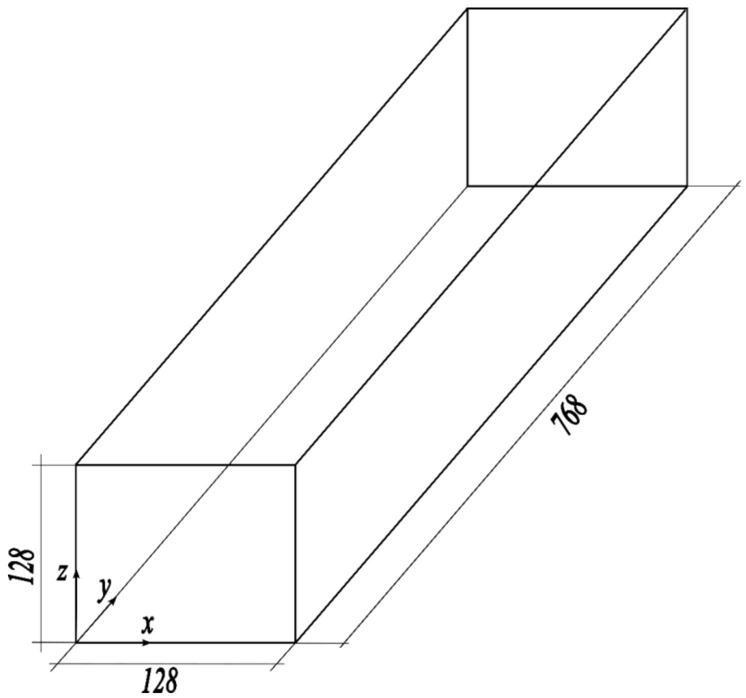

Figure 2. **Schematic representation of the Square duct flow domain**

We used the second-order moment equations to evaluate the second-order moments related to the strain rate tensor Π:

$$m_{xy}^{(2)} = 2\rho_I \Pi_{x,y,I} \tag{14}$$

$$m_{yy}^{(2)} = \rho u_{jet}^2, \tag{15}$$

$$m_{yz}^{(2)} = 2\rho_I \Pi_{z,y,I} \tag{16}$$

Where: $\Pi_{\alpha\beta,I} = \sum_I \hat{f}_i H_{\alpha\beta,I}^{(2)}$ and the subscript "I" refers to the incoming particle.

3. RESULTS

For the flow entrance of the square duct, a force was considered $\mathrm{F} = 5 \text{ x } 10^6$ where F is the pressure gradient in the streamwise direction, which is given by:

$$F = -\frac{dp}{dt} = \frac{4\rho u^2}{H} \tag{17}$$

Where $H = 128$ is the height of the simulation domain.

The results obtained through the simulation of turbulent flow take into account the average velocities, so it is necessary to carry out a high number of time steps to obtain a reliable average. For this reason, the simulation was carried out with 2 million time steps, which is sufficient to ensure that the results obtained do not vary significantly beyond this range.

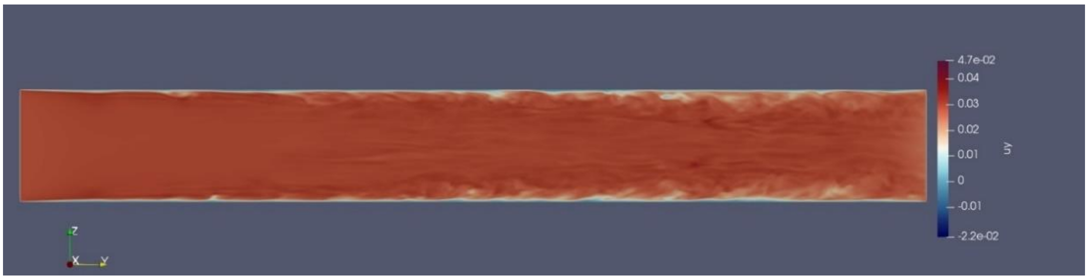

Figure 3. **Velocity field of a Square Duct Re = 20000**

The mean centerline velocity goes halfway along "X" and halfway along "Z" and travels along all the velocities uy along "Y". The decay of the mean velocity profile runs halfway along the x-axis and 3/4 of the way along the y-axis, covering all velocities uy along z.

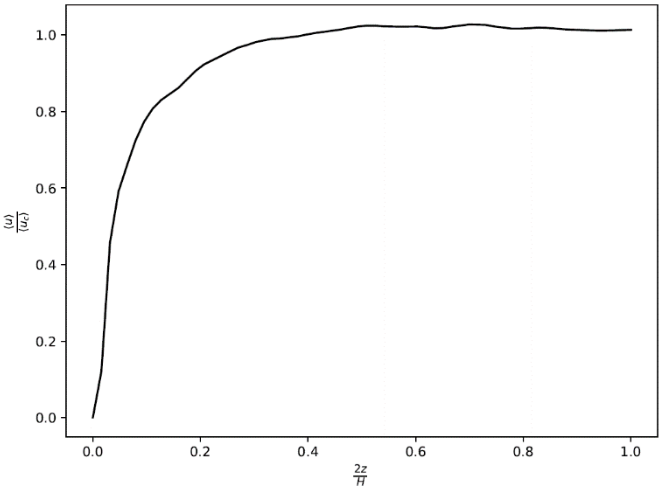

Figure 4. **The mean streamwise velocity $\langle u \rangle$ scaled by time-averaged mean streamwise velocity $\langle uc \rangle$ distributed along the half normal direction $2z$ / H with different dimensionless grid sizes**

4. CONCLUSION

Lattice Boltzmann method has been used to simulate a Square duct flow simulation in unsteady and steady state. The results were in good agreement with the analytical solutions presented during the work to validate the method used. The lattice Boltzmann method on a D3Q19 lattice model and a BGK collision operator for Re = 20000 and the reconstruction of the second-order moments for the regularized particles of the distribution function showed robust stability for the DNS scheme and an excellent alternative for solving the Navier-Stokes equations on a mesoscopic scale and represents the unsteady and steady state of the problem very effectively. The structure of the computational model designed achieved high performance in conjunction with the resources used.

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