Viscoelastic Fluid Simulation with Lattice-Boltzmann Methods

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The Lattice Boltzmann (LB) method has established itself as a tool with growing acceptance for the numerical simulation of fluid flows. It is a novel numerical method for fluid dynamics that relies on probability distribution functions for discrete particles moving on a lattice following simple collision rules, recovering Navier-Stokes dynamics. Generally, fluids are grouped in Newtonian and non-Newtonian, depending on the relation between viscosity and shear rate. The main goal in this project is to make a detailed study of non-Newtonian fluids and compare them with Newtonian fluids results. To this end, different simulations of fluids until the convergence to the stationary fluid in a channel will be done. As well, the velocity profiles of a Newtonian fluid and a non-Newtonian one, following the Carreau model, will be analyzed.

I. INTRODUCTION

When talking about fluid motion, one rapidly comes across the Navier-Stokes equations. These equations describe how the mass, momentum, and energy of the fluid change with position and time. Anyway, some advances in the theory have made Lattice Boltzmann (LB) method to be competitive when studying complicated fluid flows, as it is the case of complex fluids, the appearance of turbulence, etc. Thus, all this project will be developed with the LB method in order to replicate the fluid flow of recent experiments on complex fluids [1].

The LB method is a modern approach in Computational Fluid Dynamics, concretely it is a discrete computational method based upon the Boltzmann equation, an analogue to the Navier-Stokes equation at a molecular level, where it describes the space-time dynamics of a statistical quantity called probability distribution function. LB method finds its origin in a molecular description of a fluid: it considers a typical volume element of fluid to be composed of a collection of particles. The local flow at each grid point is represented by a distribution function for each possible velocity value. The time is counted in discrete time steps and the fluid particles can collide with one another as they move, possibly under applied forces. The rules governing the collisions are designed such that the time-average motion of the particles is consistent with the Navier-Stokes equation [2].

Considering the discretization of the fluid, it is crucial to explain the so called DnQm scheme: the molecular description of the fluid will define certain nodes, where particles can place, and different possible connections between them. Then, based on the dimensions of the lattice involved and also on its corresponding nodes different values to n and m shall be given in order to define the desired model. For instance, D2Q9 would be a 2-dimensional structure and each particle could either go to the vertices or the center of the sides, as well as staying at the center of the square, having an overall of 9 movement possibilities (see Fig. 1).

Once the model that is going to be used along this project has been introduced, it is necessary to explain some theoretical differences between Newtonian and non-Newtonian fluids. On the one hand Newtonian fluids are the ones that viscosity remains constant, no matter the amount of shear applied. However for non-Newtonian fluids viscosity can have a dependence on the shear rate [3]. As this varying behavior is not easy to fit many models have appeared trying to relate viscosity and shear rate with experimental results. One of them is the Carreau model, where viscosity and shear rate are related by the following equation:

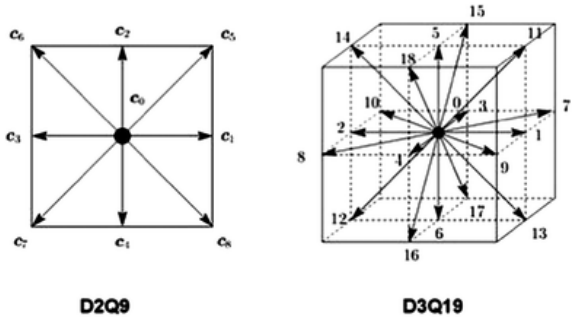

FIG. 1 Nodes and movement options of the lattice of the molecular description used in 2D and 3D simulations of LB method for the D2Q9 and D3Q19 lattices.

$$\nu = \nu_{inf} + (\nu_0 - \nu_{inf})(1 + (\lambda\dot{\gamma})^2)^{\frac{N-1}{2}} \qquad (1)$$

where ν_0 and ν_{inf} are the fluid viscosity at zero and infinite shear rate, respectively. λ is the relaxation time, $\dot{\gamma}$ is the shear rate and N is the power. An example to prove that this equation fits perfectly with experimental results is shown in figure 2. Nevertheless, in the simulations ν_{inf} was set to 0, as it was the only instance that had been implemented for the velocity inlet boundary conditions.

As a consequence of these different behaviors, their response to an applied force, or the introduction of a Poiseuille flow in one boundary of the volume shall be different, too. So the main goal in this project was to compare simulations carried out by a specific software to theoretical results. These simulations contained both

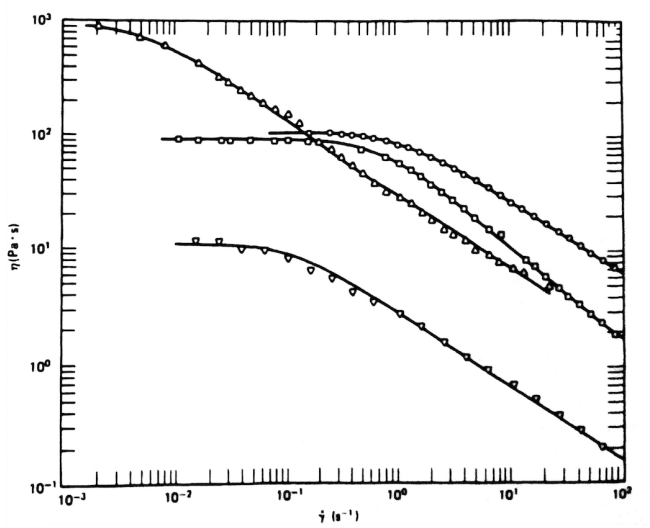

FIG. 2 Non-Newtonian viscosity of three polymer solutions as a function of the shear rate and a soap solution fitted by the Carreau equation. Reproduced from [3].

approaches: a Poiseuille flow in a Newtonian fluid and the same flow for a fluid that obeys the Carreau model.

II. METHODS

As stated before, a software was needed to reproduce the desired situation by coding. This way, two similar softwares could have been used to develop the whole project: Palabos, which was finally the chosen one, and OpenLB. These two softwares are, as its own developers define them, open-source CFD (Computational Fluid Dynamics) solvers based on the Lattice Boltzmann method. Even though the same final result should have been obtained with both of them, it was mutually agreed to work with Palabos. The main reason may be the higher level of detail provided by its user's guide, that included more theoretical references and was in general more intuitive, specially for people that are not used to working with this kind of tools.

Thus, to take a step forward it was first needed to get introduced into the programming world. First of all, many tutorials from the Palabos website had to be followed in order to understand as much as possible of the software itself and how to make use of it. All this process was vital to get into the simulation world and especially, into the Palabos world. Then, finding out what changes in the code had to be made in order to obtain the conditions for the desired experiment was the next step.

After some research and a lot of acquired coding knowledge, it was decided to simulate how two different type of fluids, Newtonian and non-Newtonian (Carreau model) behaved when a Poiseuille profile entered a 2D channel. Although many of the used parameters were dimensionless, the main idea was to simulate both experiments in a channel. Basically, this channel was build up by defining the parameter n (typically 60) controlling the number of cells. After that, there were another two dimensionless parameters (lx and ly) that were used to define the size of the simulation. This way, any value given to these two parameters, for instance lx, would mean that the size of the channel on this direction would be $lx \cdot n$ in the x-direction, equivalent to the number of cells. Finally, it was decided to take $lx = 3$ and $ly = 1$, thus the channel had a length of 180 cells and a height of 60 cells, so it would look alike a rectangle. The real system size, and thus the physical width of each cell, is implicitly determined by the Reynolds number and the specific physical parameters of the problem. This case was really interesting since an accurate theoretical solution could be obtained in the laminar (i.e. small Re) regime and compared to the simulated results. This case was really interesting since an accurate theoretical solution could be obtained and compared to the simulated results. Moreover, this comparison between both fluids would lead to the obtaining of two completely different behaviors with these conditions, confirming the theoretical calculus. Many velocity profiles and center velocities were studied in detail to fully understand the physical principle that was behind this project.

It is noteworthy to know that in both scenarios the walls were non-periodic, that is, they would not be connected to each other to keep regular flux. In addition to that, the top and bottom walls had no-slip conditions, that is, the velocity on the highest and lowest points was equal to zero. This boundary condition was implemented by means of the bounce-back algorithm [4].

The main parameters of the simulation are as follows: Reynolds number $Re = 10$, $n = 60$ and the maximum velocity of the Poiseuille flow at the boundaries $V_{max} = 0.05$. For the non-Newtonian fluid: $N = 0.5$ and $\lambda = 12000$ (which corresponds to a Weissenberg number $Wi = 10$).

After the harsh procedure of modifying the mentioned codes in order to get the wished numerical approach, the data was treated with MATLAB to acquire visible results. It was also decided to have an insight into the convergence of the codes depending on the size of the channel and the divergence from the theoretical results.

III. RESULTS

A. Simulations convergence

First of all, a research on the computational efficiency of the software was carried out changing the resolution of the simulation. Apart from studying the change in the center velocity of both fluids depending on the size of the lattice, it was also examined the minimum dimension needed to achieve an acceptable simulation error with respect to the analytical prediction of the velocity profile.

Surprisingly, both fluids showed a similar behavior if center velocity and simulation error were analyzed for growing n. Nevertheless, the results obtained were not exactly equal and some conclusions may be obtained from this computational study.

Considering the center velocity of the fluid behavior one can observe the same tendency to the same velocity as n gets higher. However, it reaches this final value in a different way depending on the type of fluid. One can check this discrepancy in figure 3. From the graph

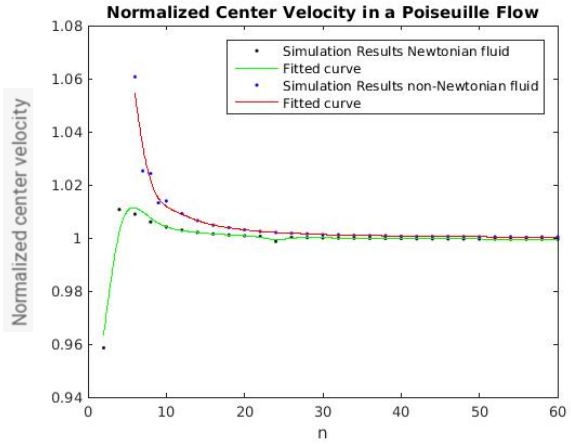

FIG. 3 Center velocity of Newtonian and non-Newtonian fluids as a function of n. In the case of the latter, the minimum n was 6 due to simulation issues.

it might seen a pretty reliable tendency to the definitive velocity, not requiring a high value of n. In contrast, not only the non-Newtonian fluid's velocity for lower n is much distinct from the tendency value than the Newtonian one, but it also does not achieve a significant convergence until $n = 20$. On the other hand, Newtonian fluid reaches a difference of 0.05 from $n = 10$ to be seen in an smoother graph. Finally, it's worth mentioning the convergence for very low values of n: in spite of getting results with the Newtonian case, the Carreau adapted model seemed to be divergent until $n = 6$, fact that evinces the higher complexity of the model itself. The fitting curves don't suit any specific function type due to the fact that their behavior isn't a common structure. Nevertheless, they were plotted just to observe an overall tendency.

Another aspect concerning center velocity could be how precisely it approaches a theoretical value. In order to do that, the software included a command that allowed to compute an RMS (Root Mean Square) error that provided a way to check the accuracy of the simulations. To make this clear, the error compares the simulated values with those theoretically found and then calculates its RMS.

From figure 4, one could notice that both models are pretty accurate to their respective theoretical result,

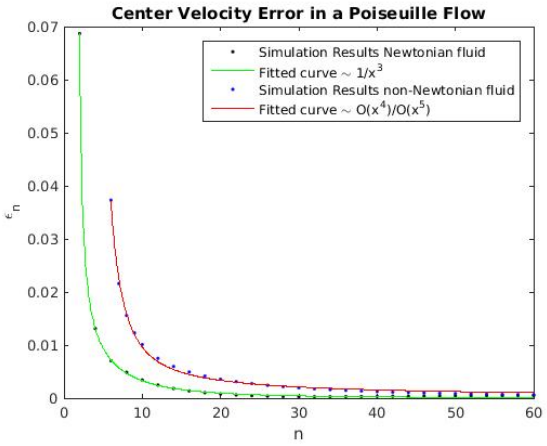

FIG. 4 Error for a Newtonian fluid as a function of n, chosen from 2 to 60 as well.

since the error becomes rapidly really small. Whereas the error in the Newtonian case decreases faster, it takes a slightly higher number of n for a non-Newtonian fluid to be precise enough. Both fitting curves share a common element: they are rational functions that tend to 0 when $n \to \infty$ but having different polynomial degrees. Despite this tendency, there's a tiny marginal increase of the error by $n = 40$.

B. Velocity profiles

As explained in section II, the main objective is the comparisons of Newtonian and non-Newtonian fluids responses to a Poiseuille profile. In principle, once the simulation is done, the velocity profile of these two type of fluids should be quite different. Basically, the Newtonian fluid profile should be much peaked than the non-Newtonian one due to different dependence of viscosity on the local shear. The resulting profiles, obtained in the center of the box ($x = 90$) and all along the y-axis, are plotted in figure 5.

Once both simulations had been run, the second goal of the work was to provide a clear vision of the response to a Poiseuille flow by a non-Newtonian fluid changing the λ parameter of the Carreau model. This parameter is a microscopic relaxation time of the fluid, which affects the tendency of the fluid to reach an stationary state after an applied disturbance. As a result, in figure 5 is seen that for a lower λ the fluid tends to resemble the behavior of a Newtonian fluid.

C. Transient of the flow

Additionally, another difference between these two types of fluids arises when speaking of convergence to the final steady flow. Although in both cases there is a

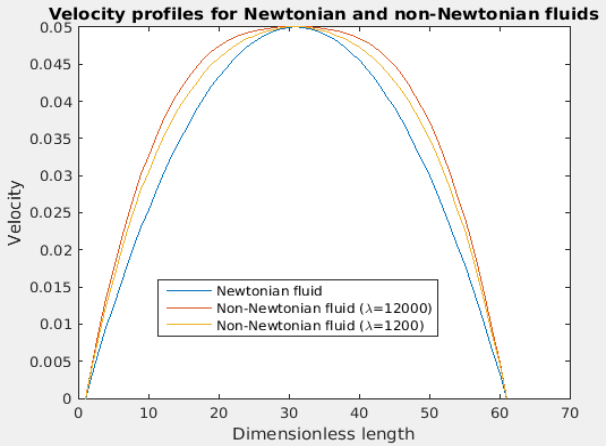

FIG. 5 Comparison of the velocity profiles between Newtonian and non-Newtonian fluids simulations, and between non-Newtonian profiles changing λ.

transient where velocity is not so stable, when some stability is reached it appears a difference since Newtonian fluids tend to achieve a constant velocity after some iterations whilst non-Newtonian ones keep oscillating during a much longer transient around a more or less defined velocity value, as seen in figure 6.

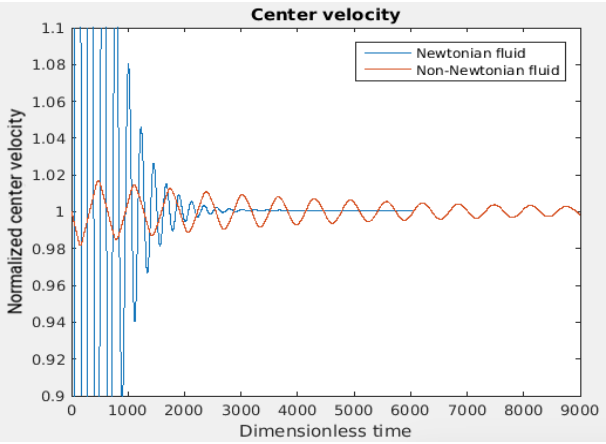

FIG. 6 Transient evolution of fluid's center velocity for Newtonian and non-Newtonian fluid.

Also, some outcomes of the simulations for the Newtonian fluid were recorded and can be observed in figure 7. From the images one could hypothesize about the compressibility of the fluid. Despite the fact that there is a flow of velocity, it is not constant, what would mean that the fluid itself is compressible. Instead, a non constant flow may indicate that it actually is uncompressible. This could also be related to figure 6, since their initial oscillations may be produced by stationary waves created at the beginning. Finally, it's worth mentioning that notwithstanding the quick convergence of the Newtonian fluid, the non-Newtonian one has a larger transient, probably due to the factor λ introduced as a relaxation time.

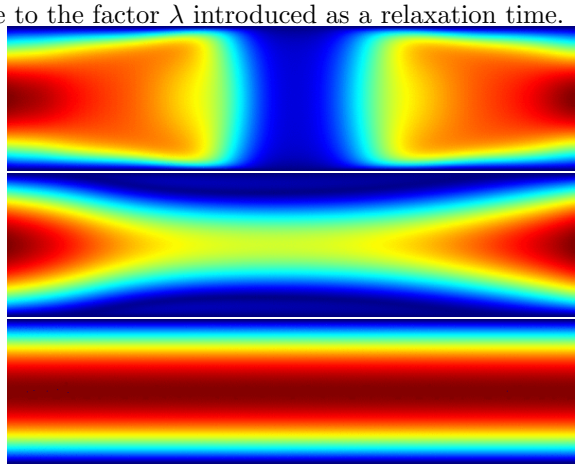

FIG. 7 Simulated Newtonian fluid response to a Poiseuille flow over time. As represented, the warmer the color, the greater the modulus of velocity in that point.

IV. CONCLUSIONS

As a result of all the insight into the Lattice Boltzmann method it is more than justified the reason why this model is gaining an increasing interest for treating fluid flows. As stated in section I, this method appeared in order to simplify some fluids problems. Moreover, it has been shown that it is very stable and that by following some simples procedures one can simulate many situations as complex as desired.

As well as a great knowledge of Lattice Boltzmann method, an incredible insight into fluids field has been achieved. From all simulations the theoretical differences between Newtonian and non-Newtonian fluids were demonstrated throughout this work.

Finally, in a more personal way, along this project a lot of new knowledge has been acquired as it involved many new aspects never treated before. One of the most enriching parts for our hypothetical professional future was when this project was first tackled, talking in terms of getting used to the software field, so necessary in simulations environment. All this project was a discovering process for both of us. As well as learning a lot about of new parts of simulation, much more that we could imagine, a completely new world in physics was opened for us, as it is Physics of fluids.

ACKNOWLEDGMENTS

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