ON THE ACCURACY OF THE PRESSURE FLUCTUATIONS CALCULATED FROM AN LBM SIMULATION OF TURBULENT CHANNEL FLOW

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ABSTRACT

In this paper the pressure fluctuations from a simulation of turbulent channel flow computed with the D3Q19 athermal lattice Boltzmann method (LBM) are compared to those calculated by the spectral simulation of Moser et al. (1999). Special care was taken to ensure that the computational domains used in each simulation were the same in order to eliminate the effect of the domain size on the turbulence statistics. It was found that the LBM over-predicts the variance of the pressure fluctuations by as much as 7%. A number of possible causes for this over-prediction were investigated, and it was concluded that the over-prediction is most likely caused by compressibility effects since the Mach number of the LBM simulation was 0.2 while the spectral simulation was incompressible. The compressibility of the LBM was examined further by comparing the LBM results to a fully-compressible discontinuous Galerkin simulation with the same Mach number. It was determined that, while the effect of the compressibility on the pressure fluctuations was similar, the density and temperature fluctuations were very different. This is because the D3Q19 LBM does not have enough degrees of freedom to allow the temperature to vary. For this reason, it is not recommended that this LBM be used for simulations in which the effect of compressibility is thought to be important.

INTRODUCTION

The lattice Boltzmann method (LBM) has received considerable interest as a potential competitor to traditional methods for direct numerical simulation (DNS) of incompressible turbulent flows in complex geometries. This is due to its simple and efficient implementation and its scalability on parallel processing computer systems. However, this work shows that the pressure fluctuations calculated from direct numerical simulations computed with the LBM differ significantly from those computed with methods based on the Navier-Stokes (NS) equations. This paper explores the potential causes of the differences in the pressure fluctuations computed by the LBM.

Direct numerical simulations are typically performed on flows with relatively high Reynolds numbers and low Mach numbers. The smallest scale in these types of flows is the Kolmogorov length scale. Since the Kolmogorov length scale is generally much larger than the mean-free-path between molecules, the fluids in these flows can be assumed to behave as a continuum and their hydrodynamic behaviour can be modelled by the NS equations. However, statistical dynamics models, such as the Boltzmann equation, are also valid for turbulent flows. In fact, the NS equations can be recovered from the Boltzmann equation by performing a multiscale expansion (Chapman and Cowling, 1970). The reason statistical dynamics methods are not widely used is because their computational cost significantly exceeds that of finite volume or spectral-type NS solvers. The computational cost of statistical dynamics methods is higher because of the number of degrees of freedom required to describe the microscopic state of the fluid. The LBM, however, restricts the particles in the model to travel with a discrete set of lattice velocities. This considerably reduces the computational cost, which makes the LBM a more viable alternative to traditional NS solvers.

The LBM was developed as an improvement to lattice gas cellular automata (LGCA). LGCA model fluids as a set of representative particles moving on a lattice with particle interactions described by a set of collision rules. These models were able to reproduce hydrodynamic behaviour, but they suffered from a number of problems, including noise. This problem was eventually solved by replacing the representative particles in the LGCA with Boltzmann-type single particle distributions (McNamara and Zanetti, 1988), which gave rise to the LBM. It was only shown later (He and Luo, 1997) that the LBM can actually be derived directly from the Bolzmann equation.

The LBM must be rigorously validated for simulating wall-bounded turbulent flows before it can be used reliably for DNS in a predictive capacity. It can be shown, through a multiscale expansion, that the LBM is approximately equivalent to the NS equations for low-Mach-number flows in the continuum limit (He and Luo, 1997). This analysis demonstrates the solid theoretical foundation of the LBM, but the suitability of LBM for DNS can only be determined by running a simulation and comparing the results to a known solution. Fully-developed turbulent channel flow is an ideal benchmark simulation for this purpose. This is due to its simple geometry, two periodic directions, and the availability of experimental and numerical data against which comparisons may be made. In this work, a simulation of turbulent channel flow is performed with the LBM and the spectral results of Moser et al. (1999) are used as the basis to validate the LBM results.

Unfortunately, simulating fully-developed channel flow with the LBM is very computationally intensive because the LBM must be implemented on a uniform cubic lattice. Since the lattice must be cubic, the grid cannot be stretched in the streamwise and spanwise directions. This means that the fine grid resolution in the wall-normal direction (which is typically more restrictive) must be applied in the two homogeneous directions as well. Additionally, grid refinement near the wall can only be achieved using a block structured mesh. This is difficult to implement since algorithms need to be developed to handle the interactions at the interfaces of neighbouring meshes. Furthermore, these algorithms typically reduce the formal order of accuracy of the LBM. The result of these limitations is that LBM simulations of turbulent channel flow are usually significantly over-resolved in the homogeneous directions and near the centre of the channel.

In an effort to reduce the computational cost, simulations (see for example Eggels (1996), Lammers *et al.* (2006), and Premnath *et al.* (2009)) have used smaller computational domains in the streamwise and spanwise directions. However, the reduction in the size of the computational domain affects the turbulence statistics obtained. This is especially true for the pressure statistics, as the two-point correlation for pressure obtained from Moser *et al.* (1999) demonstrates that the correlation length for the pressure fluctuations in the spanwise direction is much longer than the length of the domains used in previous LBM simulations. Thus, it is possible that the over-prediction of the pressure fluctuations observed in these simulations is a result of using a computational domain that is too narrow. In order to properly validate the LBM, the computational domain size must be the same for the LBM

simulation and the database with which it is being compared.

In this work, an LBM simulation of fully-developed turbulent channel flow was performed with the same computational domain as the spectral simulation of Moser *et al.* (1999). This eliminates the effect of the size of the computational domain on the turbulence statistics and allows for a direct comparison of the pressure fluctuations.

METHODOLOGY

The LBM in this work was implemented using the D3Q19 lattice, which has 19 discrete particle velocities and three spatial dimensions. The BGK single-relaxation-time approximation of Bhatnagar *et al.* (1954) was used to simplify the collision operator in the Boltzmann equation. The wall boundary conditions were implemented using the the bounce-back method, which creates a no-slip boundary halfway between the wall node and the first node that is located within the fluid domain. The bounce-back boundary condition is formally second-order accurate provided that the flow is oriented parallel to the wall, which is the predominant direction of the flow in this simulation.

The friction Reynolds number was chosen to be $Re_{\tau} \approx 180$ in order to replicate the lowest Reynolds number simulation of Moser *et al.* (1999). This Reynolds number is in the transitional range for channel flow; however, increasing the Reynolds number would only increase the computational cost and would not affect the validation of the LBM. It is expected that the performance of the LBM does not depend on the Reynolds number provided that the full range of turbulent scales are adequately resolved.

As mentioned in the previous section, the computational domain was chosen to have the same dimensions as those used by Moser *et al.* (1999). This was done to ensure that the size of the computational domain had no effect on the turbulence statistics. This is in contrast to most LBM simulations in the literature, such as Lammers *et al.* (2006), that use a narrower computational domain in order to reduce the computational cost. Table 1 compares the streamwise and spanwise dimensions of the LBM simulation in this work to the LBM simulation performed by Lammers *et al.*. While Lammers *et al.* used a longer domain in the streamwise direction, their computational domain was four times narrower in the spanwise direction than the spectral simulation of Moser *et al.*.

The grid resolution for the LBM simulation was chosen to be $\Delta x^+ \approx 2$, which is equal to the value of the Kolmogorov length scale calculated near the wall in the simulation of Moser *et al.*. Since the LBM is implemented on a uniform cubic lattice, this grid resolution leads to a computational mesh with $1080 \times 360 \times 182$ nodes in the streamwise, spanwise, and wall-normal directions, respectively. Grid refinement by means of a block structured mesh was not implemented to ensure errors from the interface model did not confound the validation results.

Table 1. Computational domain dimensions for channel flow simulations. The dimensions are written in terms of the channel half-width. δ .

	L_x	L_y
MKM	$4\pi\delta$	$4\pi\delta/3$
Lammers et al.	16 δ	δ
Current LBM	12 δ	4δ

Since the LBM is a compressible method, the Mach number must also be specified. Since the spectral results are incompressible, it would be preferable to specify a vanishingly small Mach number. However, the time step of the LBM is linearly proportional to the Mach number, and thus the Mach number must be finite in order to keep the computational cost of the simulation reasonable. In order to minimize the computational cost, it is standard practice to run LBM simulations at a Mach number near the maximum allowable value of Ma = 0.3. A Mach number of 0.2 was chosen for this work.

RESULTS

Once the flow reached a statistically stationary state, it was integrated for an additional $tu_{\tau}/\delta \approx 60$ in order to converge the turbulence statistics. The variance of the pressure fluctuations are shown in Figure 1. A comparison of the results from the current simulation, labelled "LBM", and those found by Lammers *et al.* shows that the size of the computational domain significantly affects the intensity of the pressure fluctuations near the wall, and extending the computational domain in the spanwise direction improves the match with the spectral results. However, despite this marked improvement, the current LBM simulation still over-predicts the variance of the pressure by approximately 7%.



Figure 1. Variance of the pressure fluctuations normalised by the wall shear stress, $\langle p'p' \rangle / \tau_w^2$: • LBM; —Moser *et al.* (1999); … Lammers *et al.* (2006); —FV; …DG.

One possible cause of the disagreement between the LBM and the spectral simulation is the inferior precision of

the LBM. The LBM uses finite differences to approximate the temporal and spatial derivatives in the discrete Boltzmann equation. Only the second order terms are retained in these expansions, which introduces a truncation error that affects the spectral representation of the flow. The rate at which the error decreases with grid resolution is dependent on the formal order of accuracy. Since the LBM is second-order accurate, the error is inversely proportional to the square of the grid spacing. The spectral method, on the other hand, does not suffer from truncation error because it writes the solution as a sum of basis functions and thus the derivatives do not need to be approximated.

In order to investigate the affect of the truncation error, a channel flow simulation with the same computational domain was performed with an "in house" finite volume code (Keating et al., 2004), which is also second-order accurate, and the results were compared to the spectral and LBM results. As figure 1 indicates, the finite volume and spectral results agree extremely well. This confirms that it is possible to get good agreement for the the pressure variance with a code that is second-order accurate in space and time, provided the grid resolution is sufficient. This suggests that the difference between the LBM and the spectral results are due to either another source of error or from insufficient grid resolution. The only way to prove that the grid resolution is sufficient is to perform a grid resolution study. Unfortunately, performing a grid resolution study on the LBM simulation is prohibitively expensive. This is because a reduction in the grid resolution in the wall-normal direction (for which the grid resolution is most critical) must be applied in each coordinate direction. Thus, increasing the grid resolution by a factor of two increases the computational cost by a factor of sixteen since the time step must also be reduced to accommodate a finer grid resolution. However, it is unlikely that an increase in grid resolution would significantly improve the results since the grid resolution chosen was based on the Kolmogorov length scale that was known a priori from the results of the spectral simulation of Moser et al..

Lammers *et al.* (2006) suggested that part of the reason that the LBM predicts larger pressure fluctuations is because of the presence of spurious pressure fluctuations in the simulation. Spurious pressure fluctuations occur in LBM simulations when the stability limit is approached due to insufficient grid resolution (d'Humi'eres *et al.*, 2002). In order to determine whether or not there are spurious pressure fluctuations in the LBM simulation, the streamwise and spanwise one-dimensional premultiplied energy spectra were computed for the pressure fluctuations in the LBM and FV simulations at a distance of $z^+ \approx 60$ from the wall. This location was chosen because it corresponds to the location of the largest error between the two simulations. These spectra are displayed in figures 2 and 3.

The one-dimensional energy spectra identify the contribution that each wavenumber makes to the total variance of the pressure fluctuations. The range of wavenumbers represented in the simulation is determined by the computational grid. Since spurious pressure fluctuations are caused by numerical instability, it is expected that their wavelength



Figure 2. Streamwise one-dimensional premultiplied energy spectra for the pressure fluctuations at $z^+ \approx 60$: —LBM; ... FV.



Figure 3. Spanwise one-dimensional premultiplied energy spectra for the pressure fluctuations at $z^+ \approx 60$: —LBM; ... FV.

would be on the order of the grid spacing. Thus, if the over-prediction of the variance by the LBM were caused by spurious pressure fluctuations, the one-dimensional energy spectra in figures 2 and 3 would display a significant over-prediction by the LBM in the high-wavenumber range. However, the greatest disagreement occurs in the intermediate range (between 2×10^{-2} and 6×10^{-2}). The LBM and FV energy spectra show excellent agreement in the high-wavenumber range, which demonstrates that spurious pressure fluctuations are not present in the simulation. This also provides further evidence to support the conclusion that the grid resolution for the LBM simulation is sufficient.

The streamwise and spanwise autocorrelation functions that correspond to the one-dimensional energy spectra above are shown in figures 4 and 5. These plots indicate that the larger intensity of the pressure fluctuations of the LBM simulation in the intermediate wavenumber range has a negligible effect on the autocorrelation functions. It should be noted that the spanwise correlation function has not yet decayed to zero within a correlation distance equal to half the spanwise domain size, while the streamwise correlation function decays to zero well within the boundaries of the domain. This suggests that the computational domain used is still not wide enough to contain the largest scales of the pressure field in the spanwise direction. It also demonstrates why the variance of the pressure fluctuations is more sensitive to the width of the computational domain as opposed to the length.



Figure 4. Streamwise autocorrelation function for the pressure fluctuations at $z^+ \approx 60$: —LBM; … FV.



Figure 5. Spanwise autocorrelation function for the pressure fluctuations at $z^+ \approx 60$: —LBM; … FV.

It is also possible that the over-prediction of the pressure fluctuations by the LBM is caused by compressibility effects. As mentioned in the last section, the LBM is a compressible method, and the Mach number was chosen to be equal to 0.2 in order to keep the computational cost reasonable. Since the spectral and finite volume simulations are both incompressible, there must be some error caused by the compressibility of the LBM. To determine the effect of compressibility on the pressure fluctuations, the LBM results were compared to those from a compressible channel flow simulation with the same Mach number. These results were obtained from an "in house" code, which uses the discontinuous Galerkin (DG) finite element method to solve the compressible NS equations (Wei and Pollard, 2010). The DG results (see figure 7), like those from the LBM simulation, have a higher intensity in the near-wall region. This suggests that compressibility is most likely the cause of the large pressure fluctuations near the wall in the LBM simulations.

In order to further investigate the effect of compressibility on the pressure fluctuations, a Reynolds decomposition was performed on the data obtained from the DG simulation. The pressure in the DG simulation is related to the density and temperature through the ideal gas law. Thus, the fluctuations in the pressure can be written in terms of the fluctuations in the density and temperature as follows:

$$\langle p'p' \rangle = R^{2} \left[\langle \rho'\rho'T'T' \rangle + 2 \langle T \rangle \langle \rho'\rho'T' \rangle + 2 \langle \rho \rangle \langle \rho'TT' \rangle + 2 \langle \rho \rangle \langle \rho'TT' \rangle + 2 \langle \rho \rangle \langle T \rangle \langle \rho'T' \rangle - \langle \rho'T' \rangle^{2} + \langle T \rangle^{2} \langle \rho'\rho' \rangle + \langle \rho \rangle^{2} \langle T'T' \rangle \right] .$$
 (1)

The only terms in the Reynolds decomposition that make a significant contribution to $\langle p'p' \rangle$ are the variance of the density $(\langle T \rangle^2 \langle \rho' \rho' \rangle)$, the variance of the temperature $(\langle \rho \rangle^2 \langle T'T' \rangle)$, and the covariance of density and temperature $(2 \langle \rho \rangle \langle T \rangle (\langle \rho'T' \rangle))$. The magnitude of the variance terms (figure 6) for the density and pressure are similar, and are as much as 5-7 times larger than the variance of the pressure. This is because the density and temperature fluctuations counteract each other, as shown by the negative covariance, to produce a smaller variation in the pressure.



Figure 6. Contributions to the variance of the pressure fluctuations: $-2 \langle \rho \rangle R^2 \langle T \rangle \langle \rho' T' \rangle$; $-R^2 \langle T \rangle^2 \langle \rho' \rho' \rangle$; $-\langle \rho \rangle^2 R^2 \langle T'T' \rangle$. Each term is normalised by $\langle p' p' \rangle$.

The relationship between the pressure, density, and temperature in the LBM is quite different from that in the DG simulation. The implementation of the LBM used in this work, and those of Eggels (1996), Lammers *et al.* (2006), and Premnath *et al.* (2009), does not include temperature fluctuations. Thus, while the LBM also uses the ideal gas law for its equation of state, the pressure fluctuations are directly related to the density fluctuations. If the same Reynolds decomposition were performed on the LBM dataset, the only non-zero term would be the variance of the density $(R^2 \langle T \rangle^2 \langle \rho' \rho' \rangle)$.

The difference between the behaviour of the LBM and the DG compressible flow simulations is demonstrated in figure 7. This figure contains plots of the variance of the density, temperature, and pressure. Since the temperature is fixed for the LBM, the variance is zero. This means that, in order for the LBM to recover the same pressure fluctuations as the DG simulation, the density fluctuations must be significantly different. The plots in figure 7 indicate that the pressure fluctuations from the LBM and DG simulations match reasonably well despite the fact that the density and temperature fluctuations are completely different. Thus, for simulations in which only the pressure fluctuations are of interest, the LBM may give reasonably accurate results; however, the density and temperature will not be accurate.



Figure 7. Variance of the density (top), temperature (middle), and pressure fluctuations (bottom); \circ LBM; -DG. All quantities are normalised with inner scales.

CONCLUSIONS

In this work an LBM simulation of channel flow at $Re_{\tau} \approx 180$ was performed with the same computational domain as the one used by Moser *et al.* (1999). By using the same domain size, the effect of the extent of the computational domain was removed from the turbulence statistics to allow for a proper validation of the LBM. The over-prediction of the variance of the pressure fluctuations by the LBM was significantly reduced by expanding the computational domain in the spanwise direction. However, the error between the LBM and the spectral results was still as high as 7%. This disagreement was found to be predominantly due to compressibility effects. The compressibility of the LBM can

be reduced by lowering the Mach number, but doing this significantly increases the computational cost.

The compressibility of the LBM was analysed by comparing the results to those obtained from a compressible DG simulation. The contributions of the density and temperature fluctuations to the pressure fluctuations were analysed by performing a Reynolds decomposition on the DG dataset. This analysis showed that the density and temperature fluctuations counteract each other, which is indicated by the negative covariance of density and temperature. Since the temperature is fixed in the D3Q19 LBM, the interactions between the density, temperature, and pressure are much different. The pressure fluctuations are directly linked to the density fluctuations, and thus the density behaves differently in the LBM simulation. For this reason, the D3Q19 LBM is not suitable for simulating flows in which the pressure fluctuations may be considered important. It was also found that there are differences between the turbulence statistics obtained from compressible and incompressible simulations, even at low Mach number. One such difference is that the pressure fluctuations are stronger in the near-wall region for simulations that solve the compressible form of the NS equations.

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