Large Eddy Simulation of Turbulent Square Channel Flow Using a PC-Cluster Architecture

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Abstract. A fully developed square channel flow with a Reynolds number of $Re = 4410$ (based on bulk velocity and duct width) has been calculated using Large Eddy Simulation (LES) technique with the Smagorinsky eddy viscosity model. Results for the Prandtl's secondary motion which is turbulence-driven show good qualitative picture and are in good quantitative agreement with values from other authors. Different numerical aspects have been investigated: the size of the numerical grid, the spatial discretization scheme for convection, the time discretization with first- and second-order implicit schemes. The accuracy of the results as well as the resources required for all cases studied are compared and discussed in detail.

1 Introduction

Continuing developments in numerical methods and in computer hardware allow resource-intensive turbulence models like Large Eddy Simulation (LES) to develop from pure research activities toward a reliable engineering technology. Such a process requires the use of well-balanced between each other advanced numerical techniques like parallel algorithms, spatial and temporal numerical discretization schemes of higher order which beside their better formal accuracy should fulfill additional requirements like, e.g., being non-dissipative and non-dispersive, see [1].

However, when using combinations of advanced numerical techniques the question of how resource-intensive such techniques are, becomes important. An investigation of the resources for LES computations was performed by [4] for the channel flow between two parallel plates. In their investigation the authors point out that only few systematic investigations about numerical aspects of LES exist. The reason they see in the large computational requirements for LES.

The present study deals with the required resources for LES on the example of a square channel flow. This physical problem possesses a quite typical and sensitive to the numerical modelling secondary flow, which flow was used as a test of the accuracy for the different numerical aspects studied.

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The present paper describes first details of the numerical method used which form the necessary basis for the consequent result analysis. Then the focus is set on aspects like grid resolution, spatial accuracy of convective schemes, temporal accuracy of implicit time schemes, procedure for averaging of the instantaneous flow parameters and CPU-time requirements for a parallel algorithm running on a Linux PC-cluster.

2 The LES Model and the Boundary Conditions

The widely used subgrid model of Smagorinsky has been applied in the present flow investigation. The Smagorinsky constant has a value 0.1. Reduction of the subgrid length in the proximity of the channel walls was made using Van–Driest–damping function [3, 1].

Wall Boundary Conditions. The wall functions of Werner and Wengle [9] have been implemented and utilized. This approach assumes that the instantaneous velocity component which is parallel to the wall coincides in phase/time with the instantaneous wall shear stress. Thus there is no need in averaging in time and the value for the wall shear stress is obtained at each time-step without iterations from the local flow conditions near the wall.

Periodic Boundary Conditions. Periodic boundary conditions were used to submit the values of the three velocity components and the turbulent viscosity from the outflow boundary (plane) toward the inlet boundary of the computational domain. Before submitting the values, the algorithm first corrects the velocities in the outflow plane so that the continuity equation (and therefore the global mass flow rate) is satisfied - this is made by using a correction factor which is constant for all points in this plane. The correction is performed after each SIMPLE iteration. Such an algorithm guarantees the satisfaction of the continuity equation without the need for additional algorithmic developments as those discussed in [1] - e.g. adding a pressure-drop term or using a forcing-term in the momentum equation along the channel.

3 Details of the Investigation

3.1 The Physical Problem Studied

The fully developed air flow in a square channel with dimensions $0.25 \times 0.25m$ was studied. The length of the channel was $0.6m$, or 2.4 times the channel width (this lenght was found to be sufficiently large by comparison with a case in which the channel length was $6.0m$ but further details go beyound the scope of the present paper). The average velocity trough the cross section (bulk velocity) was $0.2704m/s$ which corresponds to a Reynolds number (based on channel width) of 4410.

3.2 The Computer Code, the Numerical Grid and the Parallel Machine

The Mistral/PartFlow–3D code [5, 8] was used for the computations. The code is based on the finite volume approach, implicit time steps, the SIMPLE algorithm for velocity-pressure coupling and second-order central-differencing scheme (CDS) for convection. No use was made of a multigrid algorithm in the present study so that there is additional potential for further increase in efficiency of the computations.

The rectangular grid used is cell-centered and consists of $144 \times 48 \times 48 = 331776$ points (together with the boundary points the total number becomes 365 000). The grid was equidistant along the length of the channel. In the cross-section a refined toward the wall symmetrical grid with aspect ratio 1.07 was used. The numerical grid was separated in 12 numerical blocks (each one consisting of 27 648 points). Each block was computed on a single processor (such a distribution of the blocks is convenient for exchange of the periodic boundary conditions - in this case the inlet and the exit planes of the computational domain belong each to a single block and therefore only two processors need to exchange the information).

Investigations presented in this paper have been performed on subclusters of 12 processors of the **C**hemnitz **Li**nux **C**luster **CLIC** (528 Intel/Pentium III, 800 MHz, 512 MB RAM per node, 2 x FastEthernet), see [10]. The calculations on the PC clusters were performed with the MPI distribution of LAM–MPI 6.3.5.

The CPU-time for the investigation (93 000 time steps) was 122 hours. The parallel efficiency achieved was 0.78. On average, 3 iterations of the SIMPLE algorithm within a time step were performed.

3.3 Time Steps, Averaging Procedure and Temporal Discretization

Initially 3 000 consequently-decreasing time steps were performed in order to allow the channel flow to obtain a fully-developed state. The time step reached after the initial iterations was $0.01s$ real (physical) time; it was kept constant during the rest of the computations. Thus the CFL number which defines the relation between the temporal and spatial discretization accuracy was equal to 0.8. This value is similar to the one usually used with explicit time methods, see e.g. [7].

The averaging process was started after the initial iterations and all mean and turbulent characteristics of the flow have been obtained after averaging over 90 000 time steps (this is similar to the procedure of [2] where 100 000 time steps are used).

With the above described time steps the total physical time for averaging was $900s$ and for this time the flow forwards 973 channel-widths. The averaging in the present investigation was done only with respect to time and no use was made of the homogeneous spatial direction along the channel.

A second order accurate implicit time scheme was used in the investigation. For the case of uniform time steps the scheme is described by the following equation:

$$\left.\frac{\partial\phi}{\partial t}\right|_{\phi^{n+1}} = \frac{\frac{3}{2}\phi^{n+1} - 2\phi^{n} + \frac{1}{2}\phi^{n-1}}{\Delta t} \quad (1)$$

A first-order accurate implicit Euler-backward time-scheme is also available in the code which was used for comparison with the scheme from equation (1), see the next chapter.

4 Numerical Results and Analysis

First, an investigation was made with the parameters set as described in the previous section; we will refer it further as case "standard". Figure 1 (a) shows the secondary flows of the time-averaged flow in a cross-section of the channel for this case. Such flow patterns, called "Prandtl's second kind of secondary motion", occur only in turbulent flows of ducts with non-circular cross-sections and are turbulence-induced, see Breuer and Rodi [2]. The maximum secondary velocity appears at the diagonal bisector (the right upper corner in the figure) and its magnitude is exactly 1.50% of the bulk velocity. This value is somewhat smaller than the value of 2% reported in [2] and the value obtained by DNS in [6] which equals 1.9%.

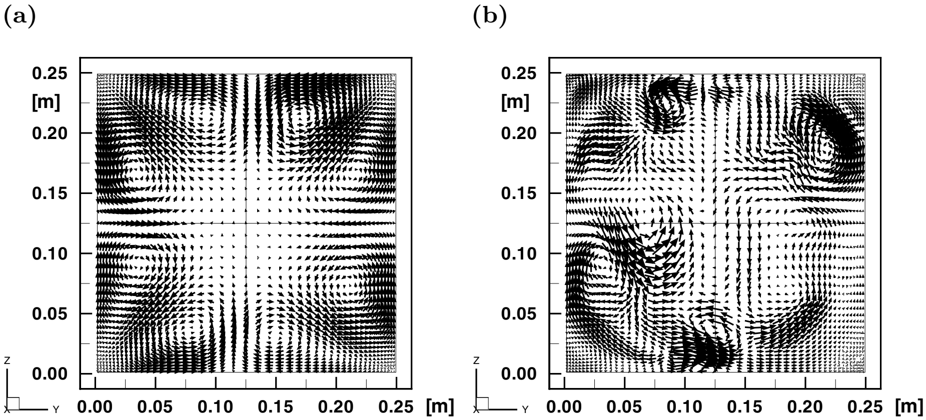

Fig. 1. (a) Secondary flows of the time-averaged flow field in a cross-section of the channel; **(b)** Instantaneous velocity vectors in a cross-section of the channel

The secondary motion is much smaller than the turbulent velocity fluctuations in the channel and consequently it can be "detected" only after averaging over a sufficiently large number of time steps. In order to illustrate this, the instantaneous velocity vectors in a cross section are plotted in Figure 1 (b). As it can be seen in the figure, no flows toward the corners are available for this particular time step. The magnitude of the plotted vectors (calculated from the velocity components which lie in the plane of the figure) is 14% of the bulk velocity, i.e. an order of magnitude higher than the averaged secondary motion.

Despite the fact that the secondary motion is quite small, it influences considerably the mean flow field - this can be seen on Figure 2 (a). The isocontours of the mean streamwise velocity show a clear deviation toward the corners of the channel. Beside this, a slight violation of the symmetry is seen on the figure. This is most likely due to the averaging process - the time for averaging might be still not sufficient to achieve perfect symmetry even after 90000 time steps. In order to clarify the effect of averaging on the symmetry of the secondary flow motion, the picture resulting after averaging over 20000 time steps is shown in Figure 3 (a).

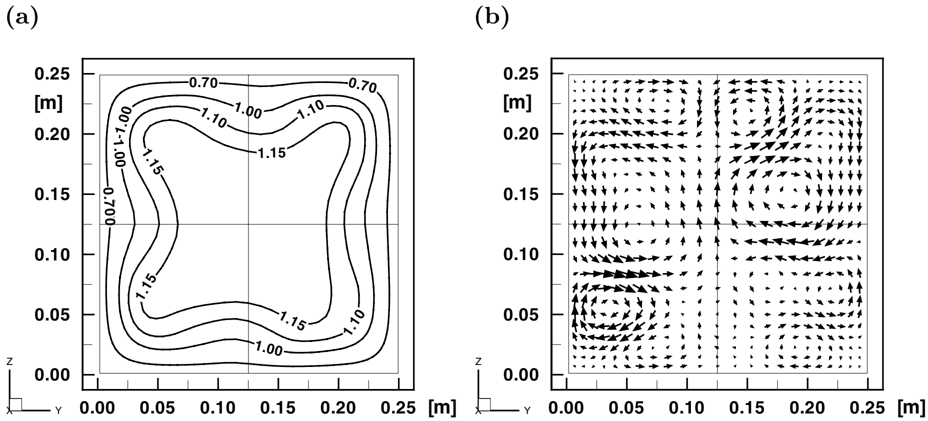

Fig. 2. (a) Isocontours of the mean streamwise velocity in a cross-section of the channel; **(b)** Secondary flows resulting on a two times coarser along y and z coordinates grid

In order to clarify the influence of the space discretization scheme for convection, a separate run was made with a first-order upwind discretization scheme. The result: no secondary motion was observed at all. The upwind scheme even damped out the turbulent motion after approx. 4000 iterations and the streamwise velocity then exhibits an “laminar” velocity profile (with a maximum of 1.78 times the bulk velocity in the middle of the channel).

The influence of the time discretiztion scheme was also investigated. A first-order accurate implicit Euler-backward time-scheme was tested for comparison. The time step for this numerical test was set exactly equal to the time step of the second-order scheme ($0.01s$). Again, as in the case of upwind spatial discretization scheme, no secondary motion was observed at all together with a “laminarisation” of the flow. A second solution with the first-order time-scheme was obtained - but now with a 10 times smaller time step, or, $0.001s$ real time. We will refer this case as “time_1st_ord”. The result from this solution (again averaging over 90000 time steps) is shown in Figure 3 (b). The maximum magnitude of the secondary motion appears in the vertical wall bisector (vertical plane of symmetry) and is 4.3% of the bulk velocity. The magnitude of the secondary

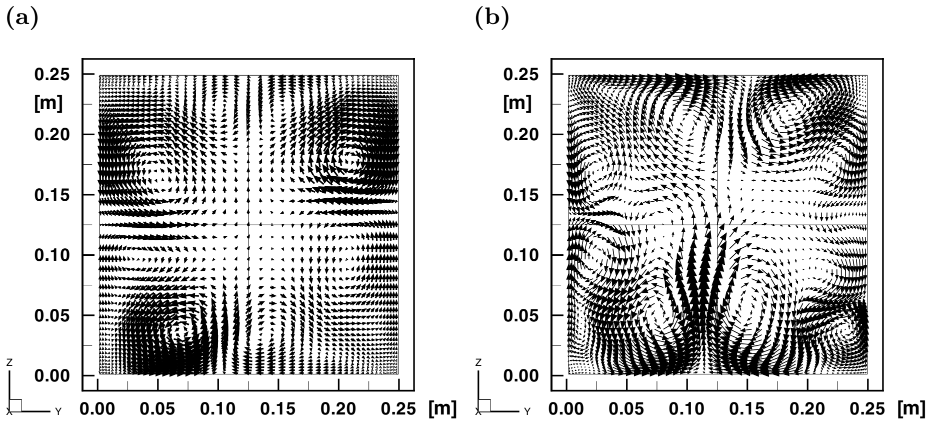

Fig. 3. (a) Secondary flows averaged over 20 000 time-steps only (compare with Fig. 1 (a)); **(b)** Secondary flows with first-order time-scheme and a 10 times smaller time-step

motion in the right upper corner is 2.4% of the bulk velocity. However, as it can be seen in the figure, the flow patterns are still deviating from symmetry which means that the time of averaging in this investigated case was not sufficient.

The influence of the grid density was also studied. Figure 2 (b) shows the results regarding the secondary motion on a two times coarser numerical grid in the cross section, consisting of ($144 \times 24 \times 24 = 82944$) numerical points. This case is refered as “min_cvs”. The observation of the instant values in the monitoring point during computations show that real turbulent oscillations of all calculated quantities were present only during about 50% of the time of the computations (but changing alternatively with periods of “laminarisation”). Consequently, after averaging, the maximum magnitude of the secondary motion is quite low - only 0.64% of the bulk velocity. Good symmetry is still not reached despite that both the time step and the number of iterations for averaging were the same as for the regular (finer) grid.

Table 1. Comparison of the calculation time for the different cases

case studied	SIMPLE iterations per time-step [approx. average value]	calculation time [hours]	relative time compared to case “standard” [%]	parallel efficiency of the calculations [-]
standard	3	121.9	100	0.777
min_cvs	2	26.7	22	0.812
time_1st_ord	2	107.4	88	0.779

Table 1 shows a comparison of the total time for the calculations (CPU-time + communication-time) for the investigated cases. As expected, the 4 times smaller amount of control volumes in case “min_cvs” requires approximately 4 times smaller time for the calculations. The 10 times smaller time step for case "time_1st_ord" leads to a smaller number of iterations per time-step and to a decrease of the calculation time. However, one should keep in mind that for this case the physical time for averaging was 10 times smaller, and, as shown above, the results are much less accurate indicating the need for a greater number of iterations with a possible further decrease in the chosen time-step.

5 Conclusion

Many numerical aspects for LES of the fully developed square channel flow have been investigated on an implicit time marching code. Accuracy of all aspects has been compared in respect to the obtained secondary flow motion. The following main results are obtained:

– **Accuracy of the numerical scheme for convection.** The second-order accurate Central Differencing Scheme showed good agreement for the magnitude of the secondary fluid motion with values from other authors. When first order Upwind Differencing Scheme (UDS) was used, no secondary flow was obtained together with a full damping of the turbulent oscillations;
– **Accuracy of the time discretization scheme.** Second order time-scheme delivered good results with a time step of $0.01s$. Such time step is suitable also for explicit time marching as for it the CFL number is equal to 0.8. First order accurate time scheme with the same time step has been found to behave as poor and nonphysical as the UDS. Even when a 10 times smaller time step was used, first order implicit Euler-backward time-scheme delivered less accurate results than the second-order scheme;
– **Accuracy of different grid resolutions.** Results with a numerical grid which was two times coarser along the two axis which lie in the cross section of the channel showed less accuracy together with a damping of the turbulence oscillations during approx. 50% of the time. However, secondary motion was still obtained with this grid and the time of the calculations was reduced to 22% which means that investigations with only 82944 control volumes might be used for quick initial testing of LES;
– **Accuracy of different time for averaging.** Differently long physical time (or, which is the same - different number of time steps) have been used to obtain the average values of the velocities and turbulent characteristics of the flow. Accurate results have been obtained only after a quite long averaging process - 90000 time steps equal to 900 seconds physical time (for this time the fluid passes a distance equal to 973 channel-widths).

The resources required on a parallel Linux PC-cluster are presented and discussed in detail for all studied cases. They present important information for the reader interested in planning and carrying out similar numerical studies exploring the power of LES. Computations of the order of 4 till 5 days on a PC-cluster of 12 computers allow presently LES to be more and more involved in industrial flow predictions.

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