PARALLEL SIMULATION OF TURBULENT FLOW IN A BACKWARD-FACING STEP

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Abstract. *The adiabatic three-dimensional turbulent flow over a backward-facing step has been studied using the Finite Volume Method and parallel processing techniques applied to the incompressible Navier-Stokes equations. The aim of the work is to explore the use of a less expensive solution, such as parallel processing in Beowulf Clusters, to solve weighted CFD cases . The classical flow over backward-facing step is a benchmark for new fluid dynamics codes due to the fact that, despite its simple geometry, it presents a very complex generation of three-dimensional structures, influencing the transition phenomenon and properties such as characteristics frequencies of vortex emission and re-attachment length. Based on the step height (h) and the free stream velocity (U_0) the flow was simulated at Reynolds 5,100 for an expansion ratio of 1.20. According to the literature, backward-facing step flow having such characteristics presents a critical Reynolds number around 748. It was employed a Large Eddy Simulation methodology with the Classical Smagorinsky model, added the van Driest damping function to the near wall eddy-viscosity. Topological results of the flow are presented, identifying Kelvin-Helmholtz instabilities during the transition period. Results for the re-attachment length were around 6.7h, for velocity and for the Reynolds stress tensor profiles presents good agreement against experimental data and validate the parallel developed code.*

Keywords*: Parallel Processing, Backward-Facing Step Flow, Turbulence Modeling.*

1. Introduction

Turbulent flows with attached and detached regions are common in Engineering applications in both internal and external flows such as diffusers, combustors and channels with sudden expansions, around airfoils and buildings. In these situations, the adverse pressure gradient or the geometry force the boundary layer to detach from the wall and then, the flow might reattaches later forming recirculation bubbles. To simulate this complex flows leads to the use of very fine meshes and small time steps, fact that can extend the required CPU time. Parallel processing may be the solution for this costly cases.

The backward-facing step, with its simple geometry can generate all the phenomena described above. Furthermore, experimental and numerical data are vastly documented for values of reattachment length, Strouhal number, Reynolds stress tensor, mean velocity, and pressure coefficient. Thus is the test case adopted here to validate the code.

Kuehn (1980), Durst & Tropea (1981) and Ötüngen (1991) studied the effects of expansion ratio ($ER = H/(H-h)$) on the reattachment length (X_R) and they found that X_R increases as ER grows. Armanly *et al.* (1983) studied the Reynolds number effect on the reattachment length and observed that X_R even grows until reaching Re=1,200 (based on the step height *h* and free stream velocity U_0). In the range $1,200 < \text{Re} < 6,600$ the reattachment length remains constant. Some inquires about the Kelvin-Helmholtz instabilities and its transition has been performed. Silveira Neto *et al*. (1993) have made a detailed topological description of the flow structures behind a backward-facing step, identifying coherent structures with characteristic frequencies. Friedrich and Arnal (1990) also studied the backward-facing step flow by using Large-Eddy Simulation. A fine statistic analysis using Direct Numerical Simulation was done by Le, Moin and Kim (1997) that obtained excellent agreement with experimental data of Jovic and Driver (1994). The Reynolds number was 5,100 and the authors have presented profiles of mean velocity, Reynolds stress tensor, reattachment length, pressure coefficient and characteristic frequencies. The experimental data of Jovic and Driver (1994) are used to validate the parallel simulations in the present work.

The Direct Numerical Simulation (DNS) can capture every scale presented in the flow but demands very fine meshes and high order schemes to do that. The Large-Eddy Simulation (LES) diminishes the mesh refinement by modeling the small scales of the flow, thus describing a more bulk flow behavior. Furthermore, LES presents excellent description of free shear flows, but it has difficulties on reproducing the near wall flow. Damping functions, as van Driest, can be employed to solve the excessive near wall eddy viscosity produced by the algebraic LES models, improving its performance in the description of flows with both wall and free shear flow regions. On the other hand, the Reynolds Average Navier-Stokes method (RANS) has been used successfully used to simulate boundary layer flows, but it can not simulate detached and very transient flow structures.

The aim of the present work is to evaluate the Large-Eddy Simulation of the backward-facing step flow at Reynolds number 5,100 using parallel processing to validate the numerical code developed and share some information about parallel processing using Beowulf Clusters. Results for velocity and Reynolds stress tensor profiles, reattachment length, pressure coefficient and flow structures are presented.

2. Mathematical Modeling

2.1. Computational Domain

The computational flow domain used is shown in the Fig. 1. The domain consists of a streamwise length $L = 30h$, including a inlet section $X_i = 1h$, vertical height $H = 6h$ and spanwise width $W = 4h$, where h is the step height. The coordinate system is placed at the lower step corner, from which the reattachment length X_R is measured.

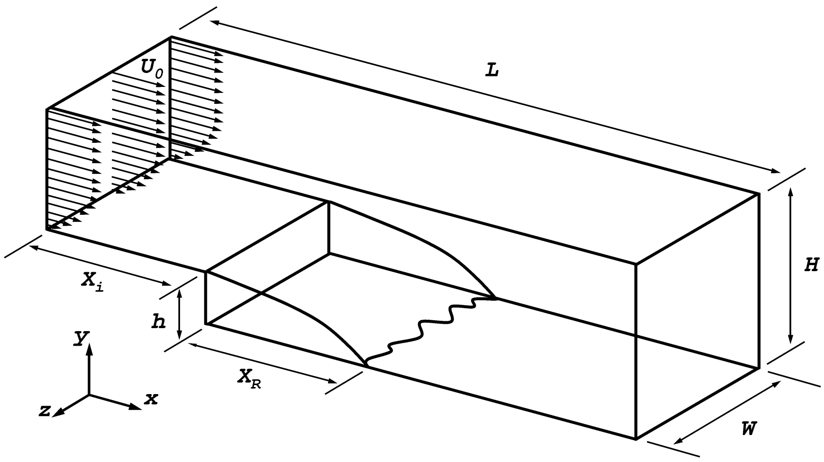

Figure 1. Schematic view of the flow domain.

The expansion ratio is 6 and the Reynolds number is defined by:

$$\mathrm{Re} = \frac{\rho U_0 h}{\mu} = 5{,}100. \tag{1}$$

The employed mesh is non uniform in the y direction and constant in x and z directions. A total of 384 computational cells are used in the x direction and 64 cells in the z direction. In the vertical direction, it is used 96 cells with non-uniform distribution, with 36 cells placed within the step ($y < h$). The grid spacing in wall units are $\Delta x^+ \approx 17$, $\Delta z^+ \approx 14$, $\Delta y^+_{\min} \approx 3$ and $\Delta y^+_{\max} \approx 50$, based on the inlet boundary layer shear velocity.

2.2. Numerical Method

The flow is modeled by the incompressible filtered Navier-Stokes equations, applying the Large-Eddy Simulation with the Smagorinsky model:

$$\frac{\partial(\rho\bar{u}_i)}{\partial t} + \frac{\partial(\rho\bar{u}_i\bar{u}_j)}{\partial x_j} = -\frac{\partial\bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu_{eff}\left(\frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i}\right)\right], \tag{2}$$

$$\frac{\partial}{\partial x_i}(\rho\bar{u}_i) = 0. \tag{3}$$

The left side of Eq. (2) represents the transient and advective terms, respectively. On the right side are the pressure gradient and the viscous term and the Eq. (3) represents the mass conservation.

The μ_{eff} is the molecular viscosity plus the turbulent viscosity computed using the Smagorinsky model, Eq. (4):

$$\mu_{eff} = \mu + \rho\left(C_S\Delta\right)^2 \sqrt{2S_{ij}S_{ij}}\,, \tag{4}$$

where S_{ij} represents the strain rate tensor and the length of the filter Δ is defined as $\Delta = \sqrt[3]{\Delta x \Delta y \Delta z}$.

The Classical Smagorinsky model produces excess of eddy viscosity close to surfaces. The van Driest damping function has been adopted to correct this fail, as shown in Eq. (5):

$$C_S = C_{S0}\left(1 - e^{-d^+/A^+}\right)^2 \tag{5}$$

where d^+ is the distance from the wall in viscous wall units $\left(d^+ = du_\tau/\nu\right)$, u_τ is the shear velocity $\left(u_\tau = \sqrt{\tau_w/\rho}\right)$, τ_w is the shear stress at the wall, A^+ is a constant usually taken to be approximately 25 (Ferziger and Peric, 1999) and $C_{S0} = 0.1$ is the Smagorinsky constant.

The equations are solved using a Parallel Finite Volume code, with second order centered differences for the advective and diffusive terms and the three-time-level temporal implicit scheme. The variable arrangement is collocated, with the Rhie & Chow interpolation to prevent problems with checkerboard pressure fields and the SIMPLEC algorithm is used to the pressure-velocity coupling.

2.3. Boundary Conditions and Time Advancement

No-slip boundary conditions are applied to the bottom walls and in the spanwise direction, the flow is assumed to be statistically homogeneous and periodic condition is used. A no-stress wall is applied at the top boundary,

$$v = 0, \quad \frac{\partial u}{\partial y} = \frac{\partial w}{\partial y} = 0. \tag{6}$$

The inlet flow consist of a mean velocity profile *U(y)* obtained from Spalart (1988) on which is superimposed a white noise of maximum amplitude 1.25% U_0. The boundary layer thickness is about $\delta = 1.2h$. To the exit it is applied a convective boundary condition (Eq. (7)):

$$\frac{\partial u}{\partial x} = 0. \tag{7}$$

Pauley, Moin & Reynolds (1988) showed that, for unsteady problems, the convective boundary condition is suitable for moving vortical structures out of the computational domain. This problem has been solved applying a damping function for the u velocity at the end of the domain, according to Souza *et al*. (2002).

The time advancement using the three-time-level scheme is implicit and the time step adopted is $\Delta t = 0.01\,h/U_0$ which is five times larger then the used in the Le, Moin and Kim (1997) DNS work. The total time simulation is $t_{total} = 2500\,h/U_0$ long enough to simulate the statistical established regime, and approximately the initial $500\,h/U_0$ data are discarded in order to remove the transient from the sample. The time period used to compute the statistics is $t_{stat} = 2000\,h/U_0$, having 20000 records (one every 10 time steps).

2.4. Parallel Processing

The parallelization strategy adopted is based on the domain division and load distribution among the computers of a Beowulf Cluster. This hardware configuration has gained popularity by its high efficiency and low cost, being an attractive alternative when compared with the MPPs machines (Massive Parallel Processors), like Cray and NEC supercomputers. In Beowulf Clusters, a server machine controls the knots of the cluster through a net and assigns the tasks that each knot will do. The in-house LTCM Beowulf Cluster consists of 10 Pentium 4® (2.8GHz/1.5GbRAM) linked by a 1 Gbps network running the Linux Fedora Core 2, see Fig. 2. The MPICH parallel library and IFC compiler are used to compile the FORTRAN90 developed code.

Each machine is responsible for its computational sub-domain, and the information is shared using the MPI (Message Passing Interface). This implies in processing and memory division among the computers (Baker & Smith, 1996), see Fig. 3.

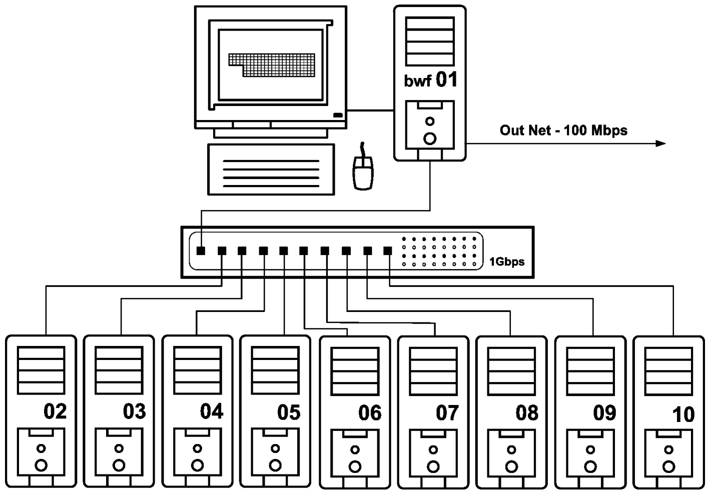

Figure 2. LTCM Beowulf Cluster, schematic view.

The parallelization of a fully implicit code imposes that the information must be shared at every time step and every linear system solver iteration. For a fully explicit formulation e.g., the information can be shared only at the time advancement. I the present work, the SOR (Successive Over Relaxation) solver is used to the momentum and the SIP (Strong Implicit Procedure) to the pressure correction equation. At each inner and outer solver iteration, the information ($\overline{u}_i$, $\overline{p}$ and μ_{eff}) is shared between the sub-domains, through the interface overlapping, see Fig. 3.

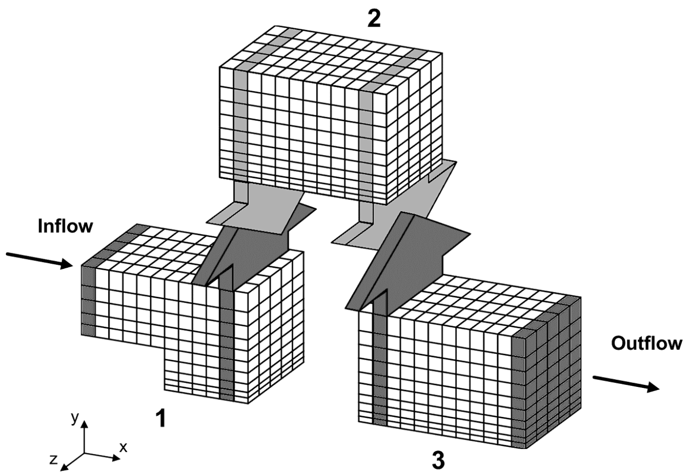

Figure 3. Parallel domain division.

The external sub-domains has the inflow (sub-domain 1) and outflow (sub-domain 3) boundary conditions of the real problem, and volumes are added to overlapping the interfaces. In the case of using 3 machines of the cluster, for example, the penultimate volume of the sub-domain 1 (a resolved volume) is introduced as inflow boundary condition into the sub-domain 2 and the second volume of the sub-domain 2 (a resolved volume) is introduced as outflow boundary condition in sub-domain 1. The information sharing between sub-domains 2 and 3 is made in a similar way. The correct and synchronized overlapping is one of the biggest issues in parallel programming.

Other important aspect in parallel processing is the choice of the convergence criteria. The linear system solvers convergence criteria and mass conservation must be respected in all sub-domains. A simple way to do that is to sum the sub-domains residues, which must be smaller than the convergence criteria. In our simulation the convergence criteria was 10^{-8} for momentum and pressure correction equations and 10^{-7} for the mass conservation.

It is possible to solve a problem using a great number of machines of the cluster, but it is important to note that the total CPU time is not inversely proportional to the number of employed machines. Some time is expended with sharing information, and that time comes large as the number of machines used grows up. The speedup definition leads to this: $S(n) = T(1)/T(n)$, where T is the time of the simulation an n the number of machines (as the mesh becomes finer, the speedup increases, because more time is expended in real work and less with sharing time).

In the present work, 3 machines has been used to simulate the backward-facing step flow. The total number of nodes is 2,359,296 and each machine is responsible for 786,432 nodes, using 503Mb of each computer RAM memory. The total CPU time was ≈216 hours, which the authors consider to be satisfactory. Probably in a serial approach, this time could be more than 540 hours (assuming a speedup of 2.5) and the memory consumption would be as high as 1.5GbRAM, or even more.

3. Results

Some results for the flow transient period, identifying the initial Kelvin-Helmholtz instabilities and the formation of coherent structures and multiplicity of scales are shown. Results for velocity and Reynolds stress tensor profiles, pressure coefficient and reattachment length are presented in stations of interest in the central plane (*z=W/2*), comparing the results of no-model and LES modeling against the experimental data of Jovic & Driver (1994).

3.1 Transient Aspects of the Flow

The Kelvin-Helmholtz instabilities are induced in the inflectional velocity profile generated by the free stream that flows over the step presenting a mixing layer behavior, see Fig. 4. The structures are shed initially in a quasi two-dimensional shape, but the transition starts quickly, as obtained by Silveira Neto *et al*. (1993). No discontinuity effects due to the overlapping occurs.

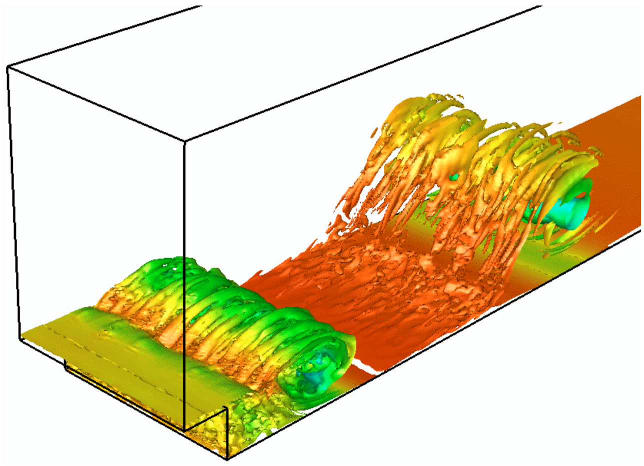

Figure 4. Iso-surface of vorticity modulus ($\omega = 1.5U_0/h$, $t = 40\,h/U_0$), colored by the pressure – LES case.

3.2. Mean Velocity and Reynolds Stress Tensor Profiles

Mean streamwise velocity U and Reynolds Stress Tensor profiles are presented in four stations of interest: in the recirculation zone ($x < X_R$, $x = 4$), close to the mean reattachment point ($x \approx X_R \approx 6$), after the reattachment location ($x > X_R$, $x = 10$), and far from the reattachment location ($x >> X_R$, $x = 19$) where the boundary layer is attached and in developing process. Figure 5 shows the nondimensional u mean velocity (U/U_0).

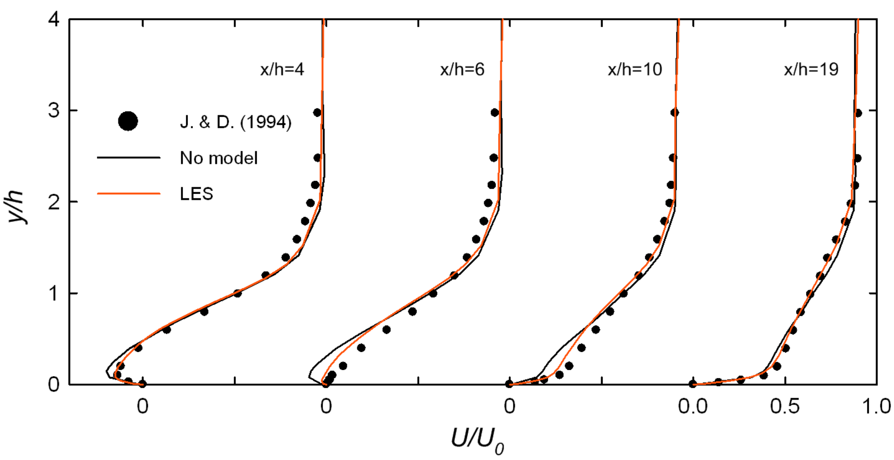

Figure 5. Mean velocity profiles.

The mean velocity presents good agreement with experimental data, especially at the recirculation zone, where the profile is practically identical to the experiment. A minor discrepancy is observed in the free stream region, with numerical data overprediction. This behavior was also observed in the DNS results of Le, Moin and Kim (1997). The $x/h = 6$ profile is underestimated, indicating that the numerical reattachment length is greater than 6.0*h*. The subsequent profiles are in good agreement despite small differences in the near wall region for the *x/h*=10 profile. The turbulence modeling plays an important role in the simulation, providing better results for the *u* mean.

The RMS profiles of the streamwise and vertical velocity fluctuations u' and v', and the Reynolds stress $-\overline{u'v'}/U_0^2$ are compared against experimental data in Figure 6.

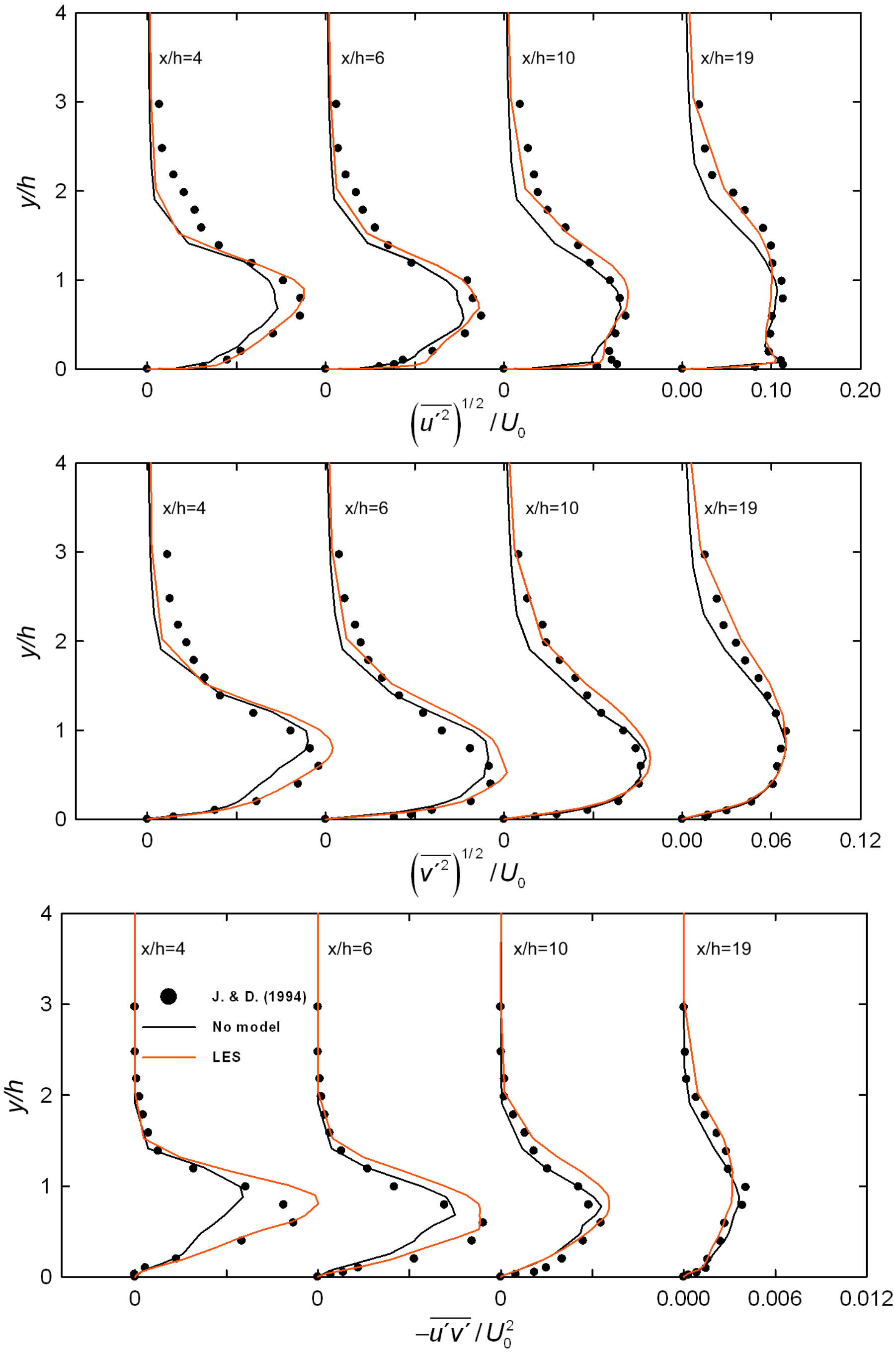

Figure 6. Reynolds stress tensor components.

There are good agreement with the experiments, with small overprediction in the vertical component that also were observed in the DNS results of Le, Moin and Kim (1997). The turbulence modeling demonstrated its importance and captured more details, especially in the $-\overline{v'u'}/U_0^2$ component, where the peak in the *x/h*=4 was captured, with under prediction for the no-model result.

3.3. Pressure coefficient and reattachment length

The pressure coefficient C_p is defined as

$$C_p = \frac{P - P_0}{1/2\rho U_0^2}, \tag{8}$$

where P_0 is the reference pressure extracted from the free stream flow. Good agreement against the experimental data is observed (see Fig. 7). There is a difference near the reattachment due to the fact that the reattachment is overestimated. In the recovery region the pressure coefficient converge to the experiment, fact that Le, Moin and Kim did not observe in the DNS simulation, where a slightly superior value for the pressure coefficient in the recovery region was obtained.

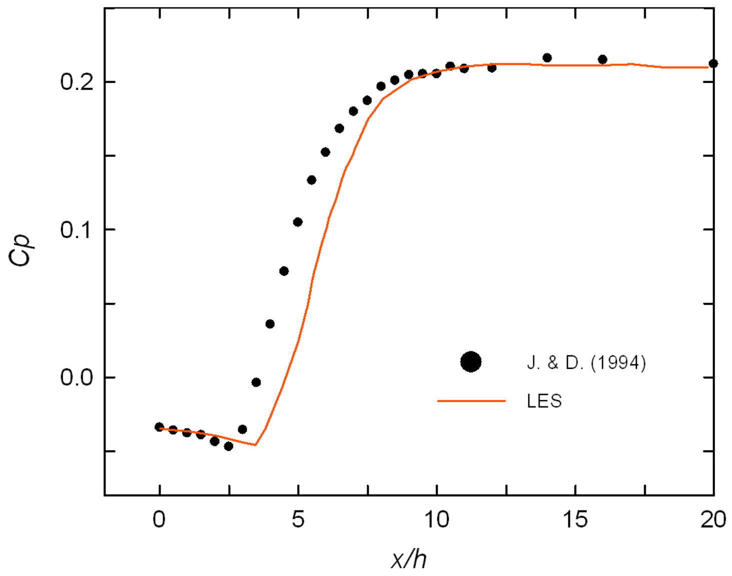

Figure 7. Step-wall pressure coefficient comparison.

The reattachment length is an important result in the backward-facing step flow that summarize in one single value the complex interactions of flow structures. The p.d.f method are used to determine the reattachment location, X_R, whose mean reattachment point is indicated by the locus of 50% forward flow fraction. The reattachment point for the LES case is $X_R = 6.7h$ and the comparison with the no model and DNS computation and experimental results are shown in Tab. 1.

Table 1. Reattachment length.

	X_R (x/h)
Exp. Jovic & Driver (1994)	6.0 ± 0.15
Le, Kim and Moin (1997)	6.28
No model	7.45
LES – Cs=0.1	6.7

The reattachment length reinforces the importance of the turbulence modeling, converging to values near the experimental and DNS data. The turbulent kinetic energy has its maximum value at the reattachment location, and in this context, a more accurate description, with Reynolds tensor close to the experimental data (Fig. 6), was obtained with LES modeling resulting in a smaller reattachment length.

4. Conclusions

The numerical simulation of a turbulent backward-facing step flow was performed in a relatively fine mesh to evaluate and validate the Implicit Finite Volume parallel code developed. Coherent structures had identified Kelvin-Helmholtz instabilities, reproducing a mixing layer behavior and the statistical results show good agreement with data of Jovic & Driver (1994). The role of the turbulence modeling was evidenced in the results of mean velocity and Reynolds stress tensor components, with small discrepancies in the reattachment zone. The reattachment length is satisfactory within 8% of agreement with experimental data.

The code presents stable behavior, without discontinuity in velocity or pressure fields by the domain division adopted, fact that can occur in an erroneous parallel code implementation. The convergence criteria established seems to be simple and practical and the linear system solvers worked well. Despite the SIP solver be of implicit approach, it did not offer resistance to parallel implementing and, in our tests, it was more efficient than others solvers like Conjugate Gradient methods.

The above conclusions has qualified the code and the LTCM Beowulf Cluster to run real large CFD problems having some millions of volumes in viable time. Furthermore, the hardware configuration used is relatively cheap and all the software needed are under GNU license.

5. Acknowledgements

The authors Cleber Spode e Aristeu da Silveira Neto thank the financial support of CNPq and Rubens Campregher the CAPES financial support.

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