Validation of an Uncertainty Estimation Approach with the Backward Facing Step Test Case

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1 Introduction

In spite of continuing progress made both in computer hardware and in simulation software, grid independent solution is still difficult to obtain in daily application, especially for 3D configuration. More and more researchers realize the importance of and the necessity for numerical uncertainty estimation. Since the pioneering work of Roache, a huge amount of effort has been devoted to this subject and important progresses have been made. Different approaches have been proposed, most of them based on the Richardson extrapolation using the concept of Grid Convergence Index (GCI) proposed by Roache [4]. All methods are expected to be able to give a correct estimation when the numerical solution is in the asymptotic convergence range. However, in real life application where the numerical solution is not always in the asymptotic convergence range, the reliability of different approaches remains to be demonstrated. A good way to validate an uncertainty estimation approach is to solve the same problem with the same mathematical model by different persons using different codes. If different results agree within uncertainty range, then the uncertainty estimation procedure can be considered as reliable.

Such attempts have been performed during the previous Lisbon Workshops. Results submitted to the first workshop showed that different results did not always agree within the uncertainty range, even for some global quantity easy to compute such as the friction resistance on the top wall for the backward facing step test case. A possible reason for such unexpected result is that all codes may not be carefully validated : implementation errors may still exist in some codes. To eliminate such kind of errors, a code verification exercise has been proposed during the second workshop by using a manufactured solution. Another reason for this discrepancy is due to the fact that the quality of the grid proposed by the Workshop organizer is not good enough. Consequently, participants of the second Workshop were encouraged to build their own grids. Surprisingly, such a procedure did not produce an improvement of the consistency of different results submitted to the second Workshop. More discrepancies were observed. One of the conclusions of the second Workshop is that, due to different numerical implementations which can not be verified in the code verification exercise using Cartesian grid, such as computation of wall normal distance, discretization of non-orthogonal terms, implementation of boundary condition, etc.., it is unlikely possible to expect that all codes give the same numerical solution even when the same mathematical model is employed.

Rather than comparing different codes, it would be more interesting to perform a self-consistency check with the results obtained with the same code. This exercise is carried out in the present study. The backward facing step test case is solved with four different grid sets using the same turbulence model and the same code. Numerical uncertainty is evaluated using the procedure proposed by Eca & Hoekstra [3]. Results are compared and discussed in the paper.

2 The Uncertainty Estimation Procedure

The uncertainty estimation procedure adopted in the paper is the procedure proposed by Eca & Hoekstra [3]. Details can be found in the reference and will not be repeated here for the sake of brevity.

Only two minor modifications are introduced by the authors of this paper.

- The first one concerns the treatment of a nearly constant solution. If the relative value of data range is less than 0.05%, we consider that the solution is grid independent. In this case, we consider that the numerical uncertainty is three times the data range.

- The second modification concerns an automatic data selection procedure. Eca & Hoekstra's approach is a least squares approach. More than three data values can be employed for uncertainty estimation. Using more than three data values is helpful when data scattering is observed. However, introducing too much coarse grid solution increases the predicted numerical uncertainty. It is desirable to include the coarse grid solution only when it is necessary. The data automatic selection procedure adopted for the present exercise is explained as follow. We perform several estimations by using different data set. The first estimation employs solutions obtained with the 3 finest grids. The next coarse grid solution is included each time. The second estimation, for example, employs the solutions of the 4 finest grids. The result of an estimation is retained as the final solution if the result is grid independent, or if the following 3 conditions are satisfied.

  1. Monotonic convergence or oscillatory convergence is observed.
  2. The order of convergence is higher than 0.5.
  3. The uncertainty level of the next estimation is higher.

  If the above conditions are not satisfied, then the last estimation including all available data sets will be used as the final result of the estimation.

3 The Numerics

Computations are performed with the ISIS-CFD flow solver developed by EMN (Equipe Modélisation Numérique, i.e. CFD Department of the Fluid Mechanics Laboratory). Turbulent flow is simulated by solving the incompressible Reynolds-averaged Navier-Stokes equations (RANS). The solver is based on finite volume method to build the spatial discretization of the transport equations. The velocity field is obtained from the momentum conservation equations and the pressure field is extracted from the mass conservation constraint, or continuity equation, transformed into a pressure equation. In the case of turbulent flows, additional transport equations for modeled variables are discretized and solved using the same principles. The gradients are computed with a least square approach based on linear polynomial or an approach based on Gauss's theorem, both ensuring a formal first order accuracy and giving a second order accurate result on a nearly symmetric stencil. Inviscid flux is computed with a piecewise linear reconstruction associated with an upwinding stabilizing procedure which ensures an second order formal accuracy when flux limiter is not applied. Viscous flux are computed with a central difference scheme which guarantees a first order formal accuracy. We have to rely on mesh quality to obtain a second order discretization for the viscous term.

4 Application to a backward facing step

The procedure described above is applied to the backward facing step test case. It is the configuration investigated experimentally by Driver and Seegmiller [1] with zero top-wall angle. The Reynolds number based on the step height, noted H hereafter, and the maximum velocity at the inlet is 50000. The channel height at the inlet is 8H. The computational domain started at 4H before the step where inlet profiles for the streamwise velocity component and for the turbulent quantities are prescribed by using an initialization program provided by the workshop organizers. The Spalart-Allmaras model [5] is employed for turbulence modelizaton. The computational domain is extended to 40H after the step where zero value is imposed to the pressure, while Neumann boundary condition is applied to other quantities. Machine zero convergence can be achieved except for transport equation for turbulent quantities due to the clipping applied to turbulent quantities to maintain a positive solution.

4.1 Meshes for different test cases

Four different type grids are employed. The first one (test case A) is a Cartesian grid (Figure 1). With this kind of topology, grid nodes are uselessly clustered in some region, making the convergence of the computation extremely difficult. The most attractive feature of this type of grid is that there is no grid quality problem. We expect that it can give a reliable reference solution. A block-structured grid is employed for the test case B. With such a block-structured topology, grid resolution in the region around the upper corner of the step is clearly not sufficient. The test case C employs an unstructured quadrilateral grid generated by the commercial grid generation software HEXPRESS. Grid around the upper corner is sufficiently refined. The last test case (test case D) uses a single block structured grid. It is the grid set A proposed by the first Lisbon Workshop organizers [2]. Each grid set contains 5-7 grids. The number of grid cells for each grid is shown in table 1.

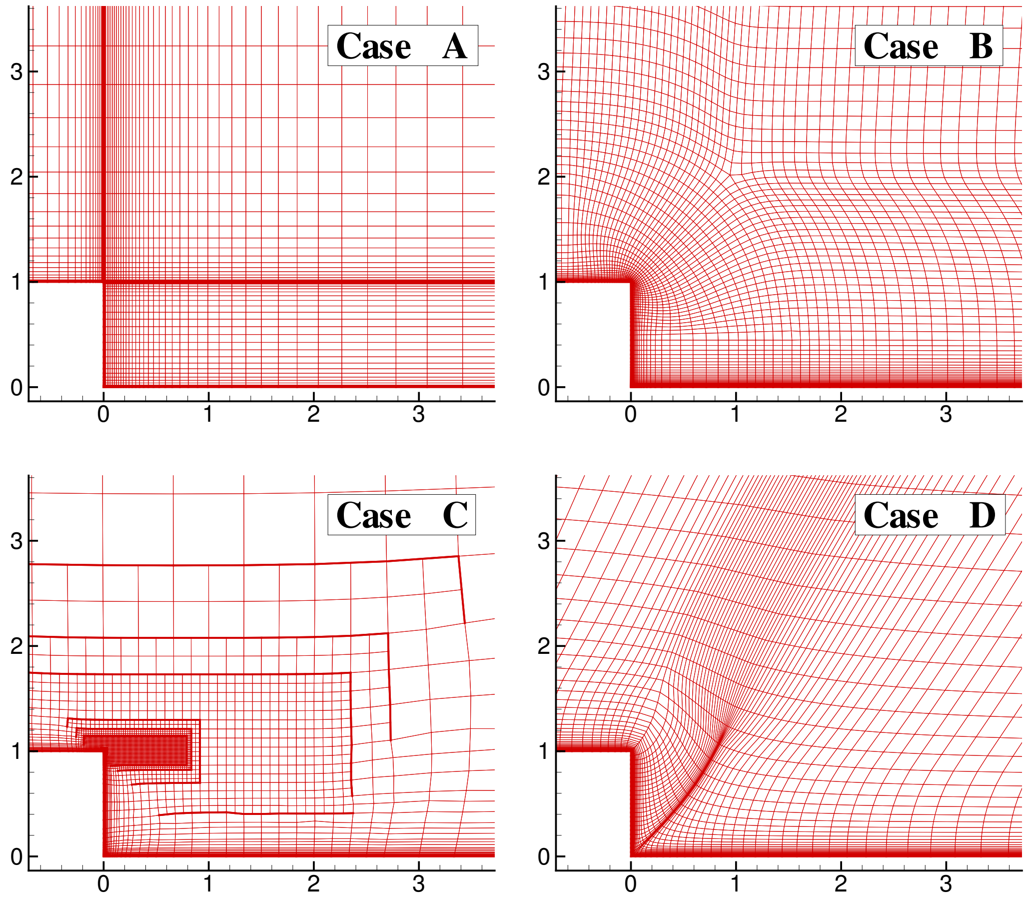

Figure 1: Mesh for different test cases.

Grid ID	Case A	Case B	Case C	Case D
Grid 1	35200	193252	95500	57600
Grid 2	28512	121582	55661	40000
Grid 3	22528	77118	26328	32400
Grid 4	17248	47838	15808	25600
Grid 5	12672	30002	7793	19600
Grid 6	8800	19110	-	14400
Grid 7	-	11715	-	10000

Table 1: Number of grid cells for different test cases

4.2 Results for global quantities

Global quantities requested by the Workshop are the friction resistance coefficient for the top and bottom wall, and the pressure resistance coefficient. Uncertainty estimation has been performed for all those quantities for all grids when at least still two coarse grids are available. When estimating the uncertainty for a grid, finer grid solution is not used. For example, uncertainty estimation for grid2 uses the result from grid2 to grid N only.

4.2.1 Friction resistance coefficient for the top wall

Figure 2 displays the results for friction resistance coefficient for the top wall. Each result is represented by a case index. Case with lower index of the same grid set is the result for finer grid. Case 5 to case 9, for example, represent the results obtained with the multi-block grid for grid 1 to grid 5. The skin friction coefficient is a quantity very easy to compute. Any two results from any data set agree within uncertainty level. Monotonic convergence is observed in all estimations with an order of convergence ranging from about 1.7 to 3.

Only one unusual observation requires further comments. While the uncertainty level for three finest grids out of four is about 0.15%, it is about 1% for the finest unstructured grid. Such a high level of uncertainty is an unrealistic result of the uncertainty estimation procedure. The estimated order of convergence for this case is 2.2. According to the estimation procedure, when the observed order of convergence is higher than 2.05, the uncertainty estimation based on Richardson extrapolation is compared with 1.25 times the data range. The highest one of these two values are considered as the numerical uncertainty. The 1% uncertainty level mentioned above is based on data range. However, the grid refinement ratio of the two grids based on which data range is computed is not taken into account in the uncertainty estimation procedure. Since we have to use a high grid refinement ratio to ensure the grid similarity for unstructured grid (grid refinement ratio of 2 between grid 1 and grid3), using data range without taking into account the refinement ratio results in an unrealistic estimation.

4.2.2 Friction resistance coefficient for the bottom wall

The result for the friction resistance on the bottom wall is shown in figure 3. Results obtained with the Cartesian grid set and the unstructured grid set agree well. Those obtained with the multi-block grid set show a good convergence behavior and a very low uncertainty level on the two finest grids. It is likely possible that these two fine grid solutions do not overlap with the fine grid solutions obtained with the Cartesian grid. However, results obtained with the mono-block grid clearly depart from the other results. We believe that the uncertainty level for mono-block grid is under-estimated by the uncertainty estimation procedure. The observed order of convergence is about 0.7. When the observed order of convergence is lower than 0.95, Richardson extrapolation tends to over-estimate the uncertainty. Uncertainty level obtained with Richardson extrapolation is compared with 1.25 times the data range. The smaller value is retained as numerical uncertainty. With the automatic data selection procedure, uncertainty estimation employs the results obtained with the three finest grids only. As the refinement ratio between grid 1 and grid 3 is only about 1.3, using data range without considering grid refinement ratio results in an under-estimation in that case.

We believe that an observed order below 1 or higher than 2 is a normal convergence behavior of a second order method when numerical error composes of a first order and a second order term, non of them being negligible. Rather than using data range for uncertainty estimation, we argue that it would be better to rely on polynomial approach. With polynomial extrapolation based on first and second order terms, the extrapolated true value is 0.001195, which is in good agreement with the expected value (about 0.0012) obtained with three other grid sets. Applying a safety factor of 1.25, the result obtained with monoblock grid agree well with other predictions within the uncertainty range.

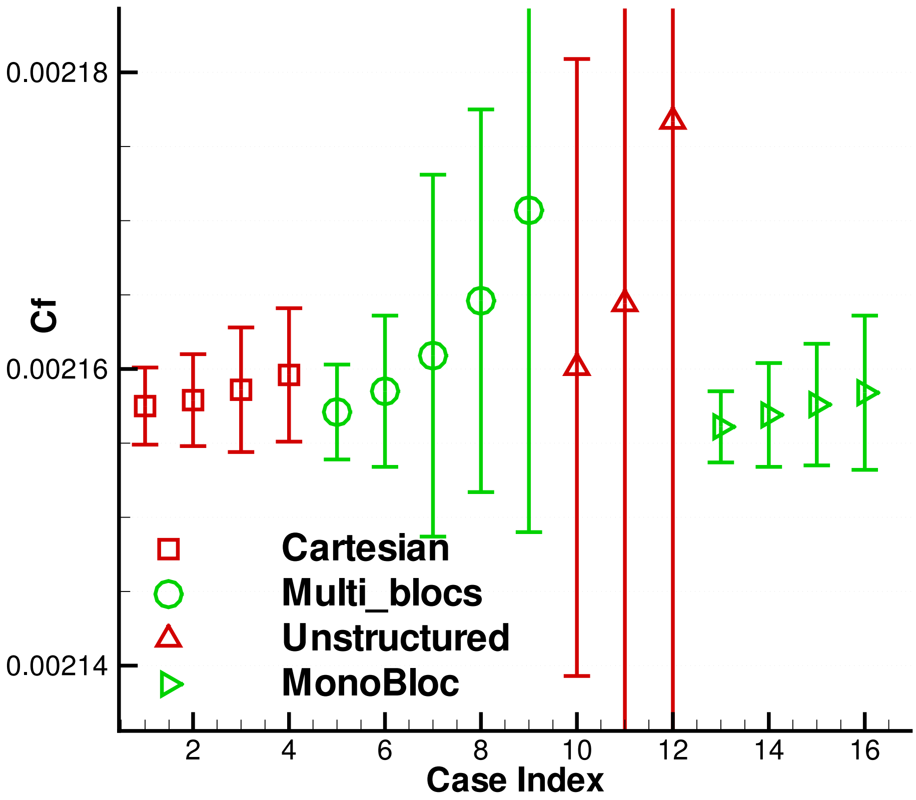

Figure 2: Friction resistance coefficient for the top wall.

4.2.3 Pressure resistance coefficient

The prediction for pressure resistance coefficient is displayed in figure 4. The predictions obtained with the Cartesian grid set and the unstructured grid set agree well within uncertainty range for any two grids. However, results obtained with the two finest grids of the multi-block grid set are located outside of the uncertainty range. As the solution exhibits a very poor convergence behavior, it is difficult to obtain an accurate estimation of the uncertainty for this case. The very low uncertainty level for the two finest grids is due to the fact that we consider that the numerical solution is grid independent, and three times data range of the three finest grids is employed as numerical uncertainty.

Once again, predictions obtained with the mono-block grid set are located outside of the uncertainty range. With a polynomial approach, the extrapolated true value is 0.206, compared to the expected true value of about 0.205 based on other results, which confirms that one can obtain an overlapping result again by using a polymonial approach.

4.3 Results for local quantities

The predicted results for the reattachement point shown in figure 5 are similar to the previous ones. All results except those obtained on the mono-block grid set overlap, at least for the results obtained with a fine grid. According to our automatic data selection

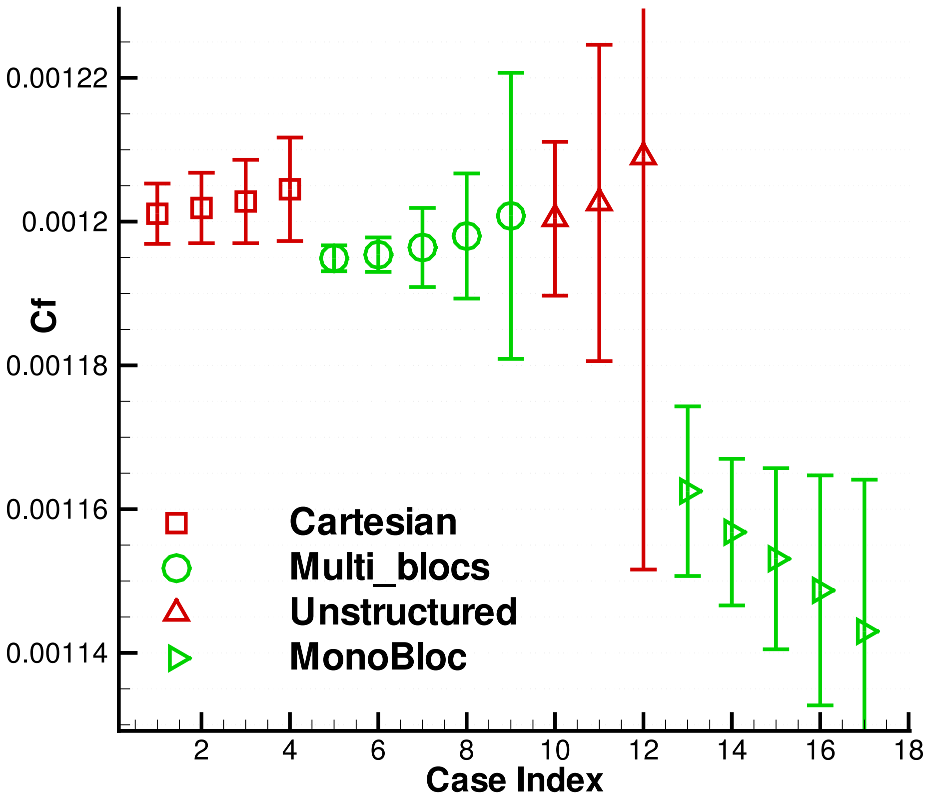

Figure 3: Friction resistance coefficient for the bottom wall.

procedure, the uncertainty estimation for the reattachement point for the finest monoblock grid is based on the four finest grid solutions which exhibit a monotonic convergence behavior with an observed order of convergence of 0.65. The extrapolated true value using a polynomial approach is 5.94H, which is not too pessimistic an estimation compared with the result (about 6H) obtained with the other grid sets. Based on this estimation, the reattachement point predicted by the monoblock grid overlaps with other solutions within an uncertainty level of about 8%.

Other results for local quantity requested by the Workshop will not be discussed here. Globally speaking, results obtained with the Cartesian grid set and the unstructured grid set agree well within uncertainty range for any quantity at any location between any two grids. It is commonly believed that reliable uncertainty estimation for numerical computation for turbulent flow an industrial application is difficult because the numerical solutions are far from asymptotic convergence range. The present study shows that it is not necessarily the case. When the grid is sufficiently refined in the location where it is needed (the upper corner of the step for this configuration), it is not so difficult to obtain a reliable estimation of numerical uncertainty.

The grid resolution around the upper corner of the step is not sufficient for the monoblock grid. Consequently, the convergence behavior of the numerical solution obtained with this grid set is poor at the position x=0 and y=1.1H. Results do not always overlap.

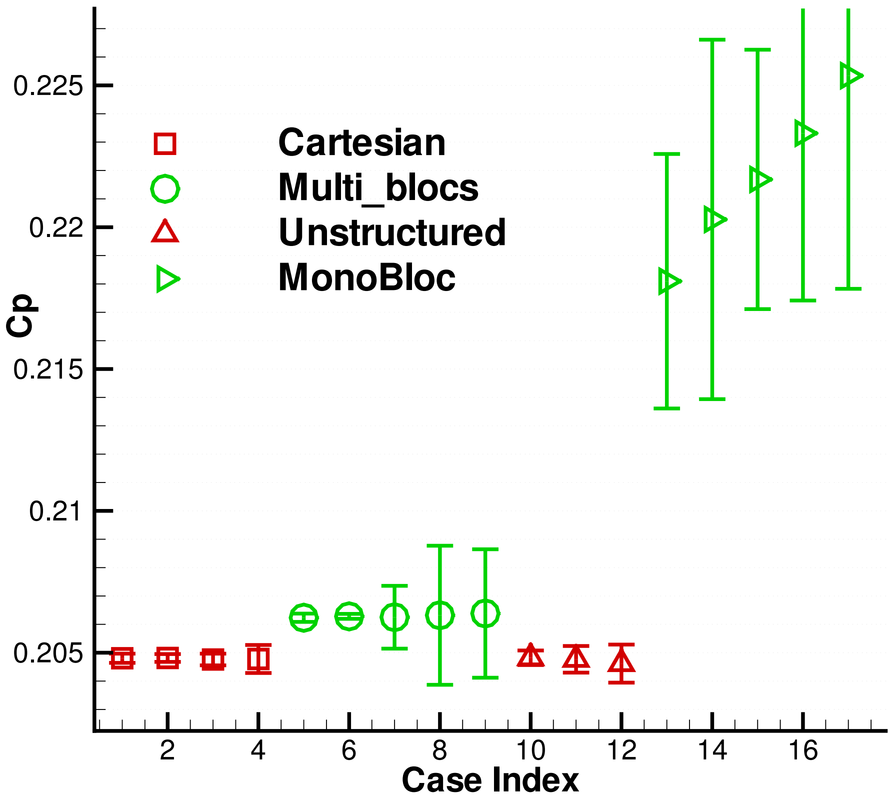

Figure 4: Pressure resistance coefficient.

Surprisingly, results obtained with the multi-block grid set do not always overlap with other results neither in spite of a better convergence behavior. At the position x=H and y=0.1H, grid quality problem near the step corner seems to have little influence. Different numerical solutions overlap at this location. At the position x=4H and y=0.1H, grid quality is good for all type of mesh. However, insufficient grid resolution near the step corner affects numerical result in this location. Poor convergence behavior is observed for some grid sets.

Only two representative results will be discussed here. The first one is the prediction of V velocity component near the step corner at x=0 and y=1.1H (figure 6). All results show a good monotonic convergence behavior, at least for the fine grid set, except for the mono-block grid set for which oscillatory divergence is observed in the uncertainty estimation for grid 2. Results obtained with the Cartesian grid set agree well with those obtained with the unstructured grid set. It is not the case for the other results. For the multi-block grid set, convergence behavior is very good. Monotonic convergence with an order of convergence ranging from 1 to 3 is observed for all grid. The non-overlapping predictions compared with the Cartesian grid and the unstructured grid is unlikely a failure of uncertainty estimation. Concerning the mono-bloc grid set, numerical predictions are far from convergence. It is unlikely possible to obtain a reliable estimation for the uncertainty for this case.

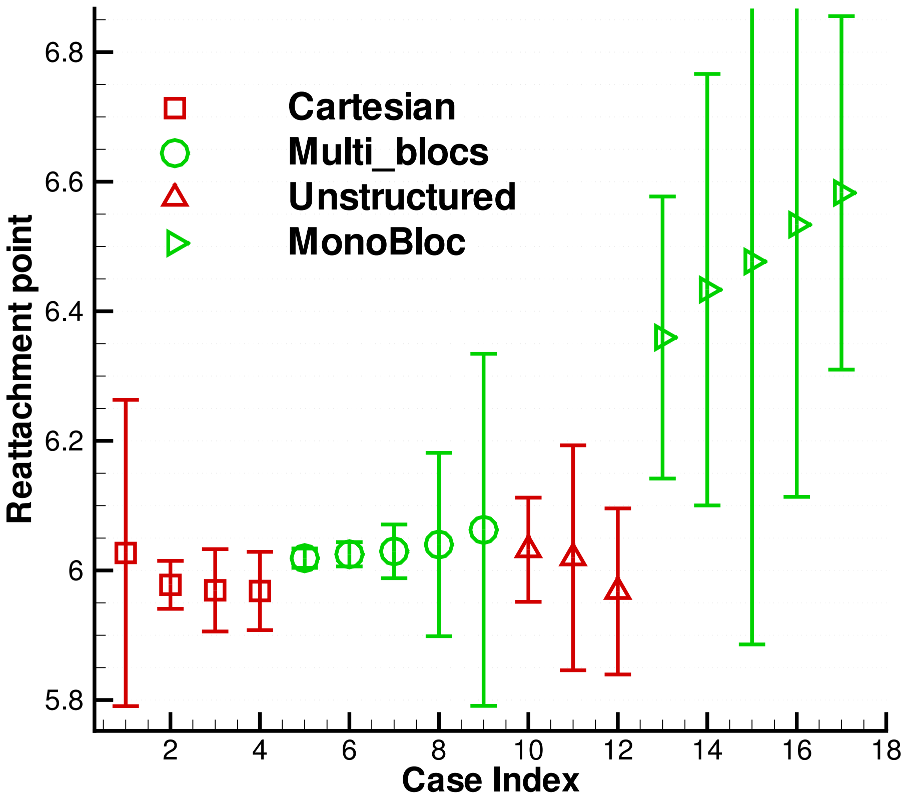

Figure 5: Reattachement point

Figure 7 compares the prediction for the U velocity component at the position x=4H and y=0.1H. A monotonic convergence with an order of 1.5 to 1.7 except for the finest grid set is observed for the Cartesian grid. Uncertainty estimation for this grid set is reliable. A very high uncertainty level is observed with the unstructured grid due to the use of data range for uncertainty estimation. The predicted value agrees well compared with the prediction obtained with the Cartesian grid. Monotonic convergence behavior with an order of convergence of 1.3 and 2.1 is observed for the two finest grids of the multi-block grid set. We believe that the uncertainty estimation for these two grids is also reliable. However, they do not overlap with the results obtained with the Cartesian grid. Results obtained with the mono-block grid set exhibit an oscillatory convergence behavior. Non-overlapping results are obtained, which leads us to believe that the uncertainty estimation for this case is unreliable.

Numerical predictions with good convergence behavior have been obtained with two grid sets, one with Cartesian grid, and and other with multi-block structured grid. However, both numerical solutions for both velocity components at two selected locations do not agree within the uncertainty level. Although the error is small, about 0.2% of the reference velocity, it is unexpected. The ISIS-CFD code has been verified with a manufactured solution during the last Lisbon Workshop. It has been shown to converge to the analytical solution of the manufactured solution for the Spalart-Allmaras model. We

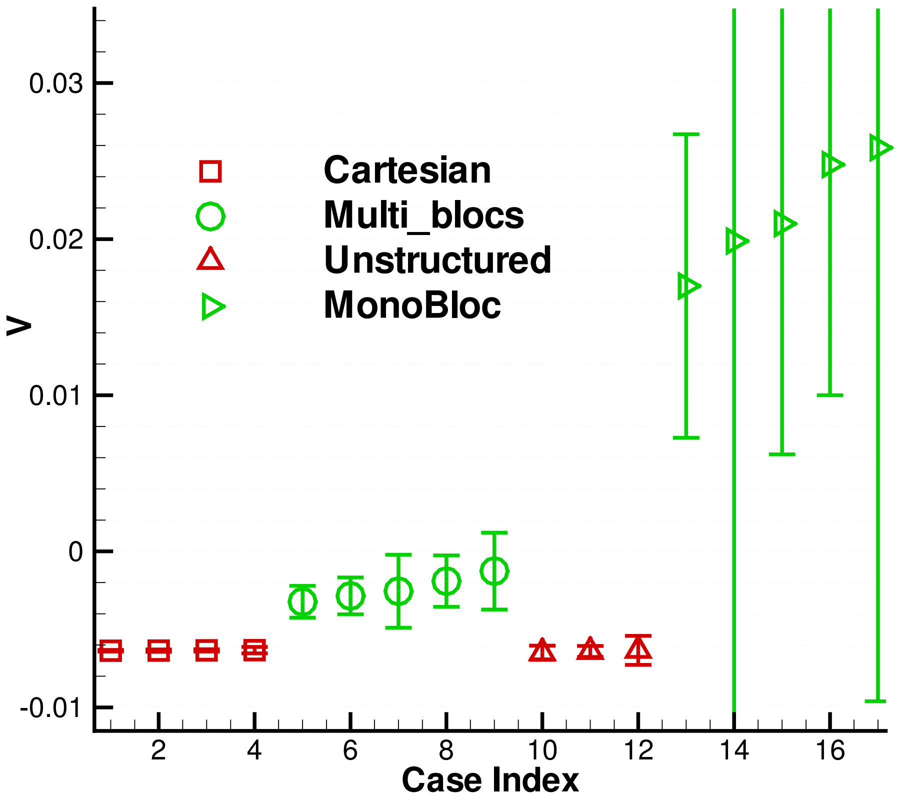

Figure 6: V velocity at x=0 and y=1.1H

expect that different computation for real problem should converge to the same solution when the grid is refined. Careful verification of the numerical solution reveals that such unexpected discrepancy is due to the numerical procedure for wall normal distance computation implemented in the ISIS-CFD code which is unable to give a grid topology independent solution. Figure 8 compares the computed wall normal distance for the finest grid of each grid set. It can be seen that the result obtained with the Cartesian grid is quite similar to that obtained with the unstructured grid, while difference can be easily observed on the result obtained with the multi-block structured grid. The difference observed in the normal normal distance computation explains the non-overlapping result found in the computation.

5 Conclusion

The backward facing step test case has been computed with four different grid sets with the same turbulent model and the same code. When the grid is sufficiently refined around the upper corner of the step, either with a Cartesian grid or with an unstructured grid, reliable uncertainty estimation can be obtained with the least squares approach proposed by Eca & Hoekstra, combined with an automatic data selection procedure adopted in the present study. It is not necessary to use an excessively fine grid to obtain a correct

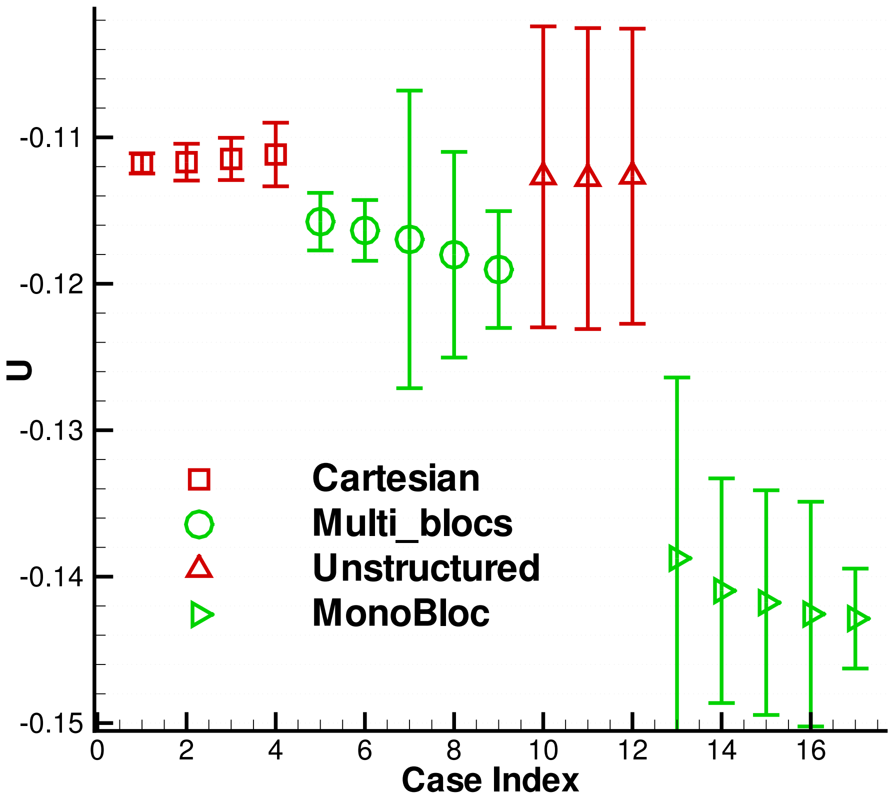

Figure 7: U velocity at x=4H and y=0.1H

estimation. When the grid is not sufficiently refined, such as the case with mono-block structured grid, uncertainty estimation become more problematic as expected. Monotonic convergence can still be obtained for the global quantities. In this case, good estimation can still be obtained with polynomial approach. When a monotonic convergence behavior can not be observed as it is the case with mono-block grid for local quantity most of the time, reliable estimation to numerical uncertainty is difficult to obtain. One of the shortcomings of the uncertainty estimation procedure proposed by Eca & Hoekstra is that it relies on data range for uncertainty estimation without taking into account the grid refinement ratio of the two grids on which the data range is computed. It is therefore recommended to take into account the grid refinement ratio when uncertainty estimation is based on data range.

6 Acknowledgments

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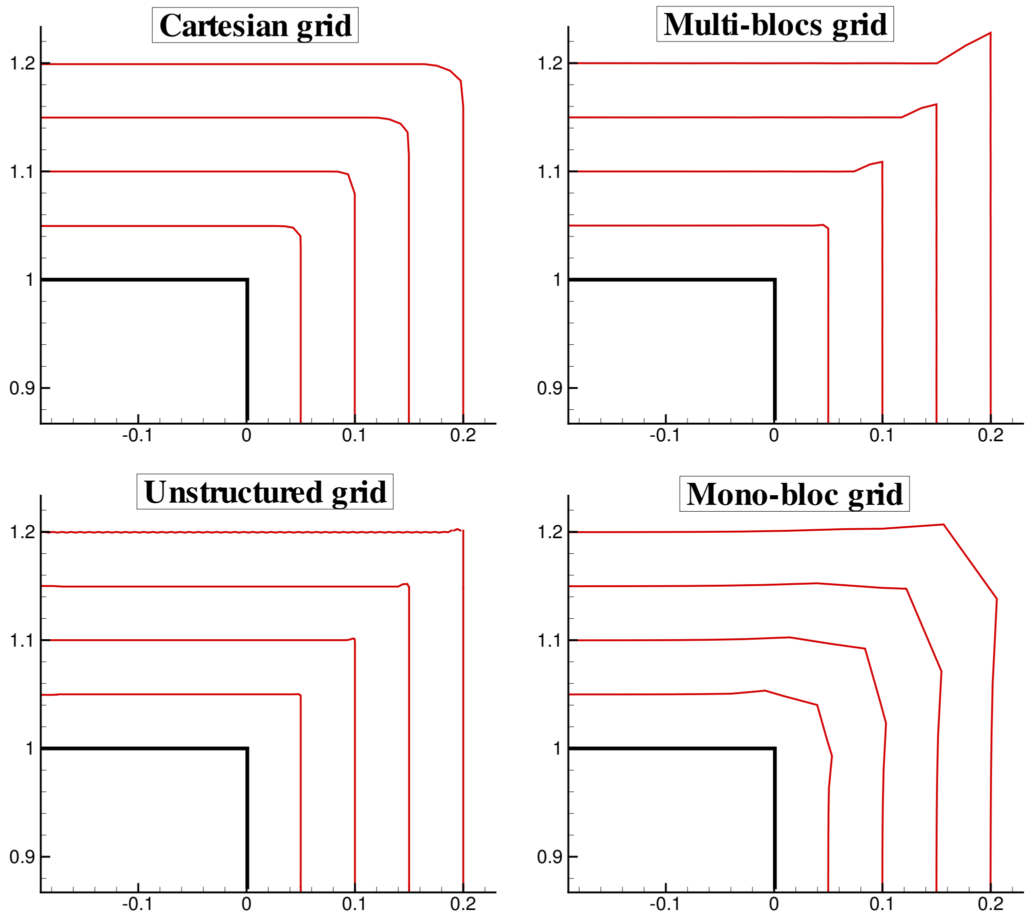

Figure 8: Wall normal distance

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