A Solution Qualification Procedure Applied to a Backward Facing Step Test Case

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1 Introduction

Method based on Richardson extrapolation using the concept of Grid Convergence Index (GCI) proposed by Roache [7] is the most commonly used approach for numerical uncertainty estimation. With a carefully designed and sufficiently refined grid set, the GCI approach can give reliable uncertainty estimation for global quantity such as resistance. However, it becomes more problematic when it is applied to local quantity. Local quantity on a systematically refined grid set usually does not exhibit a monotonic convergence behaviour. In the case where monotonic convergence behaviour is observed, the apparent order of convergence is often quite different from the expected theoretical order. In these cases, the result of the uncertainty estimation can not be consider as reliable. It depends on the ad-hoc choice of the uncertainty estimation procedure employed and the data set selected by a user. In the present paper, we propose a procedure that combines the result of error estimation for a global quantity and data difference between different grids to obtain the uncertainty estimation for a local quantity. This procedure is applied to a backward facing step test case. Different types of grid are employed. It has been found that this procedure provides not only a plausible uncertainty estimation for local quantity, but also useful information that can be used to qualify the numerical solution.

2 Uncertainty Estimation Procedure

To evaluate the uncertainty for a local quantity, we first determine the L1 norm error for this quantity using the Grid Convergence Index approach. This can be proceeded as follow. First, we choose a target region. The target region can be a simple rectangular domain inside the computational domain. Then we build a test grid in the target region. A uniform Cartesian grid is sufficient for this purpose. Next, we interpolate the solution from all grids to the test grid. In the present study, a 4^{th} order accurate interpolation method using a least squares approach is employed. This interpolated solution will be noted as ϕ^k where k is the grid index, grid 1 being the finest one. After that, we evaluate

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the L1 norm of the solution difference between the grid k and the grid 1 as:

$$Diff^k = \sum_i |\phi_i^k - \phi_i^1| \, Vol_i$$

Here, Vol_i is the volume of the i^{th} element of the test grid. Richardson extrapolation is applied to the data set $Diff^k$ to determine the estimated true value $Diff^0$ which is expected to be negative. The extrapolation procedure employed in the present study to determine $Diff^0$ will be described later in the paper. $| Diff^0 |$ can be considered as an approximation to the L1 norm error of the finest grid. For a given grid with index k, a data field is constructed by scaling the data difference with respect to the finest grid as

$$\frac{| Diff^0 |}{Diff^k} \left(\phi_i^k - \phi_i^1\right)$$

It is evident that the L1 norm of this data field is equal to the estimated L1 norm error on the finest grid. Hence, it can be considered as an approximation to the error on the finest grid. Applying a safety factor F_s according to the common practice in a GCI approach and taking into account all available solutions, the numerical uncertainty in the i^{th} element of the test grid for the finest grid solution can be approximated by

$$Max \left[\frac{F_s \, | Diff^0 |}{Diff^k} \left(\phi_i^k - \phi_i^1\right)\right], k = 2, ..., n$$

where n is the number of available solutions employed in the error estimation procedure. The value for the safety factor F_s can be 1.25 or 3 depending on the reliability of the extrapolated result for $Diff^0$. The L1 norm error for each grid can be approximated by

$$Err^k = | Diff^0 | + Diff^k$$

The extrapolation method employed in an error estimation procedure is of crucial importance. Extrapolation with unknown exponent using grid triplets is the simplest procedure. But it can not always provide a reliable estimation. The approach proposed by Stern & al. [9] takes the theoretical order of convergence of the numerical solution as an input. Our experiences show that the asymptotic order of convergence of a numerical solution may depend not only the numerical discretization scheme, but also the type of grid employed in the computation. Hence, the no theoretical order of convergence exists for a numerical solution. The least squares approach proposed by Eça and Hoekstra [3] improves the reliability of the estimation. But it is not always the best choice. We believe that the best extrapolation procedure is a procedure that adjusts itself to the data. Here is the extrapolation procedure employed in the present study. More than 4 grids are necessary. 5-6 grids are recommended. Apparent order of convergence for each successive grid triplets is determined by using the Richardson extrapolation with unknown exponent. The choice of the final extrapolation method and the selection of data set used for the extrapolation will depend on the behaviour of the apparent order of convergence thus obtained. To be able to observe the variation of the observed order of convergence, at least 5 grids are required. A abrupt variation of the apparent order of convergence gives evidence to data scattering. In this case, least squares approach based on one term Taylor series expansion with unknown exponent will be employed. Unless some coarse grid results are too coarse to be included, all available data are used for the extrapolation. When the observed order of convergence is almost the same for all grid triplets, the extrapolated result using the finest grid triplets is considered as the most appropriated estimation. Extrapolation method based on two terms Taylor series expansion with fixed exponent may be employed when the variation of the observed order of convergence is regular but not nearly constant, or if the value is too far from the expected one. Example given in the flowing section will better illustrate how this self adaptive approach is applied.

3 The Numeric

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 guarantee 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 test case

The procedure described above is applied to a backward facing step test case. It is the configuration investigated experimentally by Driver and Seegmiller [2] 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. This test case has been chosen for the two workshops devoted to CFD uncertainty analysis hold in Lisbon in 2004 and 2006 [4] [5]. 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 Lisbon workshop organizers. The Spalart-Allmaras model [8] 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 not achieved for all the cases due to clipping applied to turbulent quantities to maintain a positive solution. However, cares have been taken to ensure that iterative error is negligible.

4.1 Mesh for different test cases

4 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 resolutoin in the region around the upper corner of the step is 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 for the Lisbon Workshop [4].

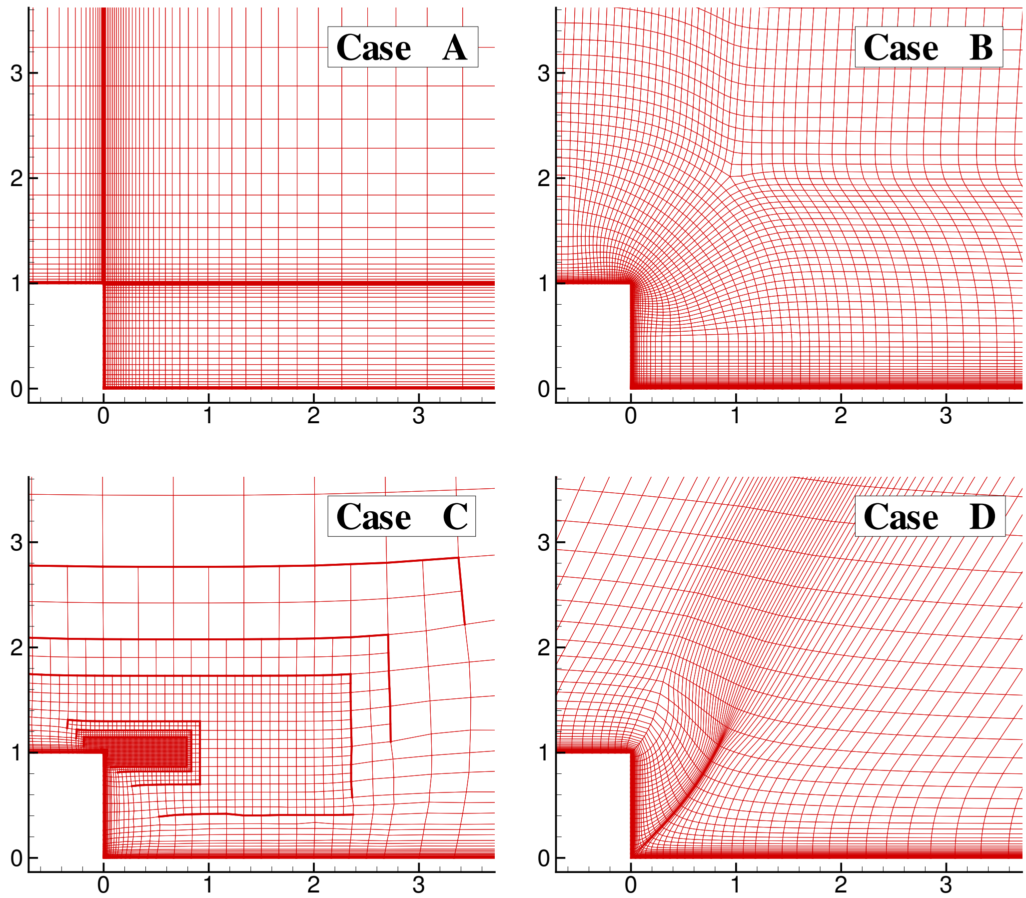

Figure 1: Mesh for different test cases.

4.2 Uncertainty estimation

The target region is a rectangular domain defined by (0.05≤x≤8, 0.05≤y≤1.5). It is covered by a 200×100 uniform test grid. Uncertainty estimation is performed with the procedure described in the previous section.

Test case A, Cartesian grid

Cartesian grid is employed for this test case. 6 grids have been employed for the computation. The divergence observed on the finest grid triplet may due to insufficient convergence on the finest grid. Data scattering is observed. But error estimation is quite reliable when least squares approach is employed except for the case with the 4 finest grids. The solution converges with second order accuracy as expected. We choose the result obtained with the least square approach using all available date (grid set 6 to 1). The estimated L1 norm error for the finest grid is Err^1=0.0039. A safety factor F_s=1.25 is applied.

Grid ID	Case A	Case B	Case C	Case D
Grid 1	0 /35200	0 /193252	0 /95500	0 /57600
Grid 2	9.60E-4/28512	3.52E-3/121582	5.41E-3/55661	0.0540/40000
Grid 3	2.00E-3/22528	7.12E-3/77118	1.72E-2/26328	0.0871/32400
Grid 4	3.62E-3/17248	1.42E-2/47838	2.93E-2/15808	0.125/25600
Grid 5	6.15E-3/12672	2.25E-2/30002	6.05E-2/ 7793	0.171/19600
Grid 6	1.01E-2/ 8800	3.33E-2/19110	-/-	0.226/14400

Table 1: Solution difference and number of grid cells for different test cases

Grid set	Case A	Case B	Case C	Case D	Case D^2
6-5-4	-0.0054/ 1.6	-0.0102/ 1.3	-/-	-1.279/0.2	-0.312
5-4-3	-0.0027/ 2.2	-0.0265/ 0.8	-0.0009/2.0	-0.489/0.5	-0.284
4-3-2	-0.0020/ 2.6	-0.0008/ 2.6	-0.0128/1.3	-1.225/0.2	-0.351
3-2-1	-/-0.3	-0.0857/ 0.2	**-0.0120/1.4**	-0.723/0.4	**-0.350**
6 to 1	**-0.0039/ 1.8**	**-0.0092/ 1.3**	-/-	-0.782/0.4	-0.324
5 to 1	-0.0037/ 1.9	-0.0080/ 1.4	-0.0082/1.7	-0.749/0.4	-0.334
4 to 1	-0.0053/ 1.5	-0.0060 / 1.7	-0.0124/1.4	-0.859/0.3	-0.351

Table 2: Richardson extrapolation results for different test cases

Test case B, block-structured grid

6 block-structured grids are used for the computation. Due to data scattering, least squares approach is the only choice. There is no particular reason to exclude any data. All available solutions are employed for the extrapolation as the previous case. The estimated L1 norm error for the finest grid is Err^1=0.0092. The observed order of convergence is 1.3, which is much lower than the expected second order accuracy. In spite of a low observed order of convergence, we consider that the extrapolation is reliable. Hence a safety factor F_s=1.25 is applied.

Test case C, unstructured grid

The 5 grids employed in this test case are generated with the commercial grid generation software HEXPRESS. There is no data scattering problem. However, the coarsest grid is too coarse. The apparent order of convergence is about 1.4. We choose the result obtained with the finest grid triplet, namely Err^1=0.0120. A safety factor F_s=1.25 is applied.

Test case D, single block structured grid

The grid used for this test case is the grid set A employed in the Lisbon Workshop. There is little variation in the apparent order of convergence. But the value is too low (less than 0.4). The type of grid and the nature of the numerical scheme make us believe that such a convergence order is unrealistic. To obtain a better estimation for the uncertainty, we employ a polynomial method with a first and a second order term in the Taylor series expansion. Results are shown in the last column in Table 2. Almost identical extrapolated results are obtained with the two finest grid triplets, which justifies the the use of the polynomial method. We choose the result obtained with the finest grid triplet, namely Err^1=0.350. Usual safety factor F_s=1.25 can be applied to this case as well.

Comparison between different test cases

The estimated L1 norm error and the apparent order of convergence for different test cases are shown in figure 2. The quality of the numerical solutions obtained with different grids are quite different, both in the magnitude of the error and in the order of convergence. Result obtained with the single block structured grid is problematic. The error level is two order higher compared with the best result obtained with the Cartesian grid. In addition, the apparent order of convergence is too low (p=0.4). It is unlikely possible that we can obtain a reliable uncertainty estimation for this case. Results obtained with the block-structured grid and the unstructured quadrilateral grid are more accurate compared with the test case D. However, the error norm is about 5 times higher compared with the result obtained with the Cartesian on the fine grid using about the same number of grid points. The order of convergence is lower than second order both for case with block-structured grid and for the case with the unstructured quadrilateral grid. For the test case with block-structured grid, the lost of accuracy might be due to the fact that grid density is not sufficient both in the region around the up corner and in the region after the step where free shear layer develops. For the case with unstructured grid, grid is intentionally refined in the above mentioned two regions. We believe that the lost of accuracy is due to the first order accurate viscous flux reconstruction scheme employed at the grid refinement interface rather than a grid resolution issue.

4.3 Uncertainty self consistency check

In this section, we compare the uncertainty estimation for different test cases to see if the error bars overlap. The solution differences with respect to the test case A together with the uncertainty level are compared at three different location x=1h, 4h and 7h in figures 3, 4 and 5 respectively for test case B, C and D. At x=1h, error bars for test case A and B do not overlap near the shear layer after the step near y=1h. This may be due to the fact that the grid set B is not sufficiently refined in this region. Similar results are observed downstream in the recirculation region at x=4h and x=7h. The failure in uncertainty estimation in this region reveals the limitation of an approach based on Richardson extrapolation. Numerical error observed in this region is convected from upstream. It is impossible to estimate the error in those region correctly using only local information. Error transport equation approach [1] [6] may be more suitable in such situation.

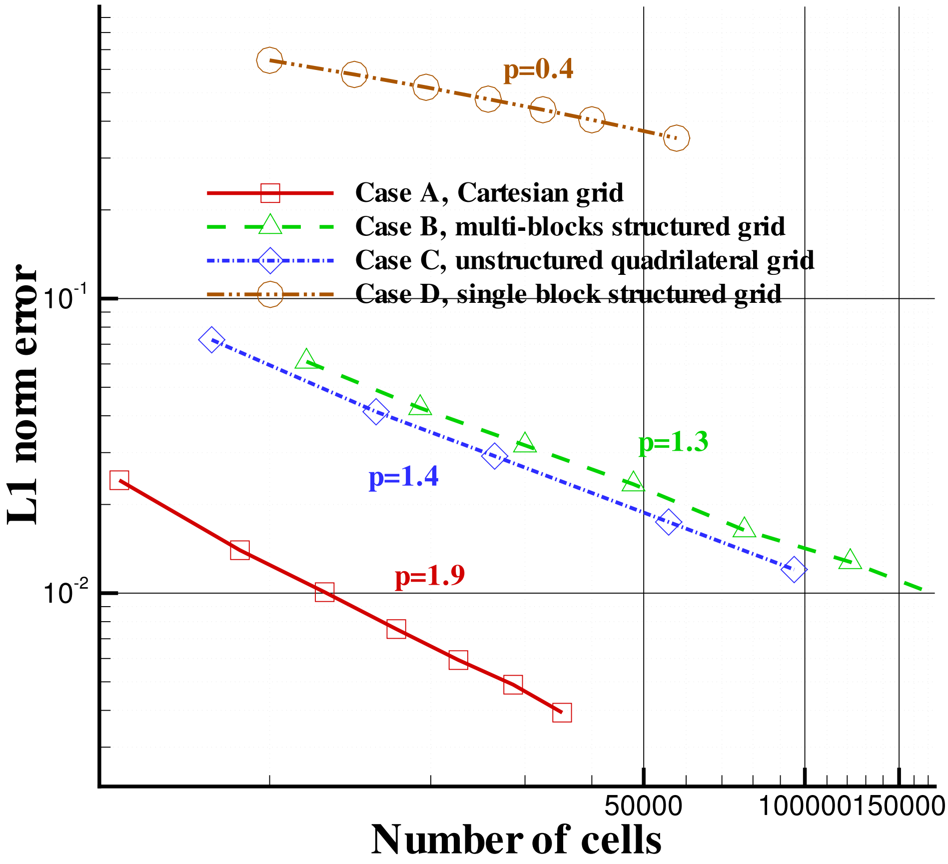

Figure 2: Estimated L1 norm error and order of convergence

For the test case A and C, error bars overlap very well at all locations. In addition, they do not excessively overlap, indicating that the level of the estimated uncertainty is appropriate. The level of the uncertainty for the test case D is about 20 times higher compared with the test case B and C. This order of magnitude is appropriate. If we had used the result obtained with Richardson extrapolation using unknown exponent, the level of uncertainty would be two times higher, which is excessive. If we had chosen a safety factor of 3 instead of 1.25 because of very low observed order of convergence (about 0.4), the uncertainty level would increase by a factor of more than 2, which is not appropriate as well. As the error level for the case D is so high compared with the case A, another possibility to check the uncertainty estimation is to consider the solution obtained with the finest grid for the case A as the exact solution and use this solution to evaluate the error obtained on the grid set D. Figure 6 displays the solution difference between the finest grid A and the finest grid D. It can be considered as an approximation to the error for the grid D. Figure 7 shows the estimated uncertainty for the grid D. It can be seen that both approximations are in good agreement. In both cases, the highest error is found in the free shear layer after the step with a maximum value of about 0.12. This observation suggests that the error estimation procedure and the choice of 1.25 as safety factor are appropriated.

In RANS computation, first order upwind scheme is still employed by some peoples

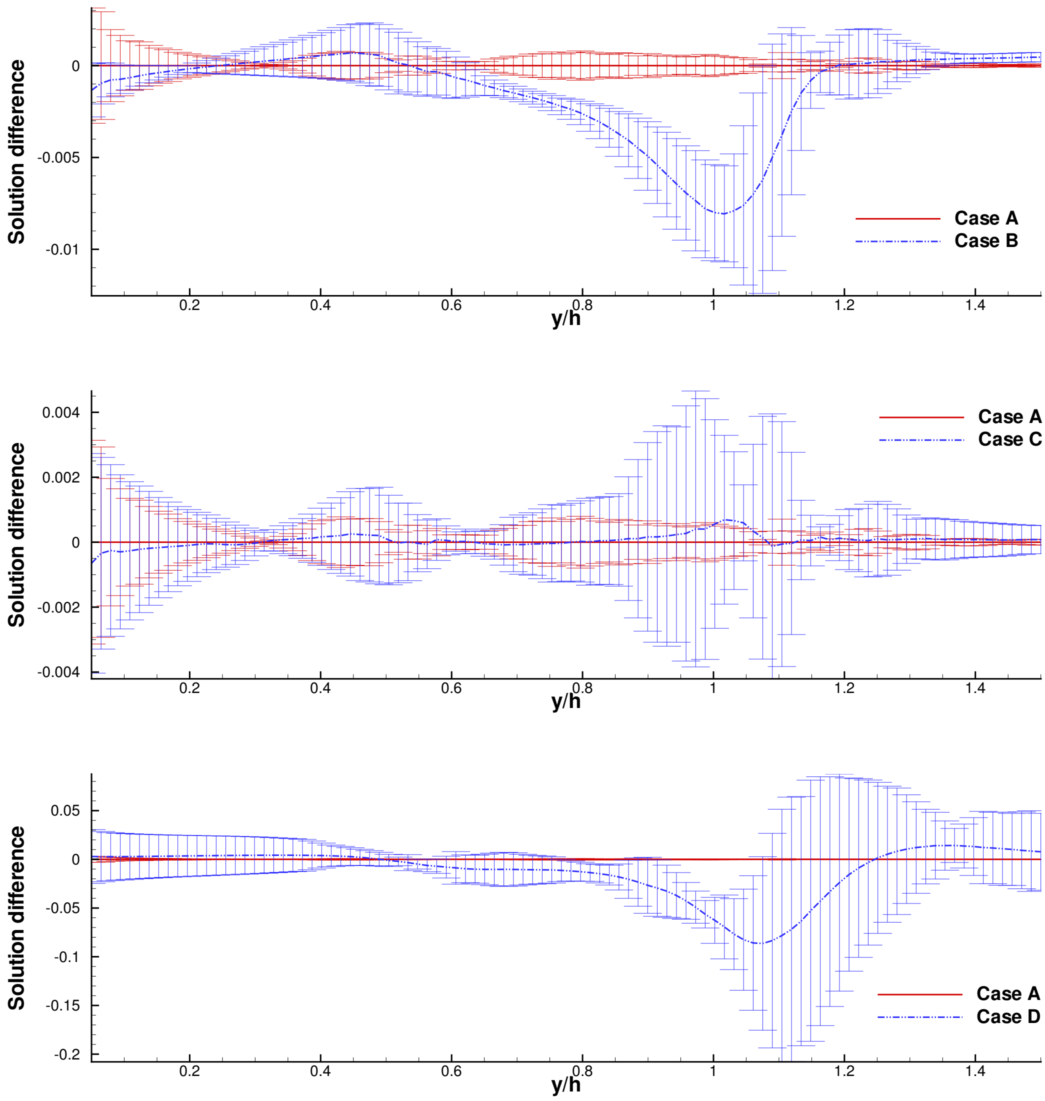

Figure 3: Uncertainty self consistency check at x=1.

in some situations for one reason or another. It is argued that such practices have little impact on the overall accuracy for practical applications. An exercise has been done in the present study to illustrate such impact, as well as to evaluate the capability of the procedure proposed in this paper as a method to qualify a numerical solution. Computations have been performed with first order upwind scheme for the transport equations for turbulent quantities with the grid set A and B. The estimated L1 norm error is shown in figure 8. When we look at the observed order of convergence, the lost of accuracy is evident. The observed order of convergence is reduced from 1.9 to 1.0 and from 1.3 to 0.7 respectively for the case A and B. Concerning the L1 norm error, the deterioration becomes more important for fine grid. On the coarsest grid, for example, the L1 norm error increases by about 90% for the case A and 40% for the case B. However, on the finest grid, it is about 4 and 3 times higher for the case A and B respectively. Figure 9 compared the numerical uncertainty for the finest grid at the x=1h, 4h and 7h for the test case A for the two computations using first and second order scheme for turbulent

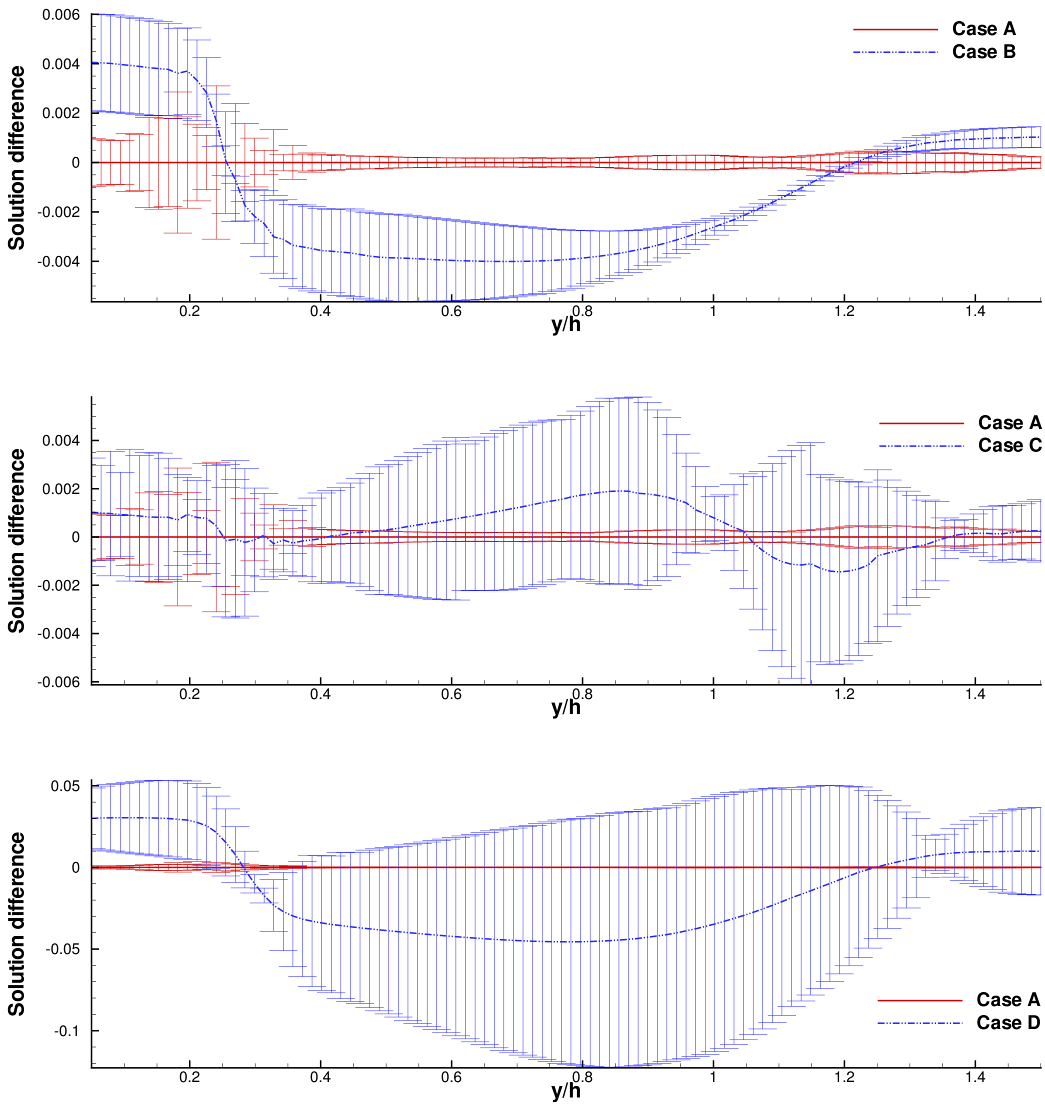

Figure 4: Uncertainty self consistency check at x=4.

quantities. Error bars overlap reasonable well most of the time. At those positions, the two solutions differ by about 0.1% to 0.5%. Such difference is quite small indeed, which justifies in some extent the use of first order scheme for turbulent quantities. However, as second order scheme can provide a more accurate solution, why it should not be always used in the computation?

5 Conclusion

In addition to uncertainty estimation, we believe that the convergence behaviour of error norms in a grid refinement study is equally important in a solution verification exercise. This procedure is commonly employed in code verification exercise using exact solution. A solution qualification procedure is proposed in this paper that allows to estimate error norms with confidence in a solution verification exercise where the exact solution is

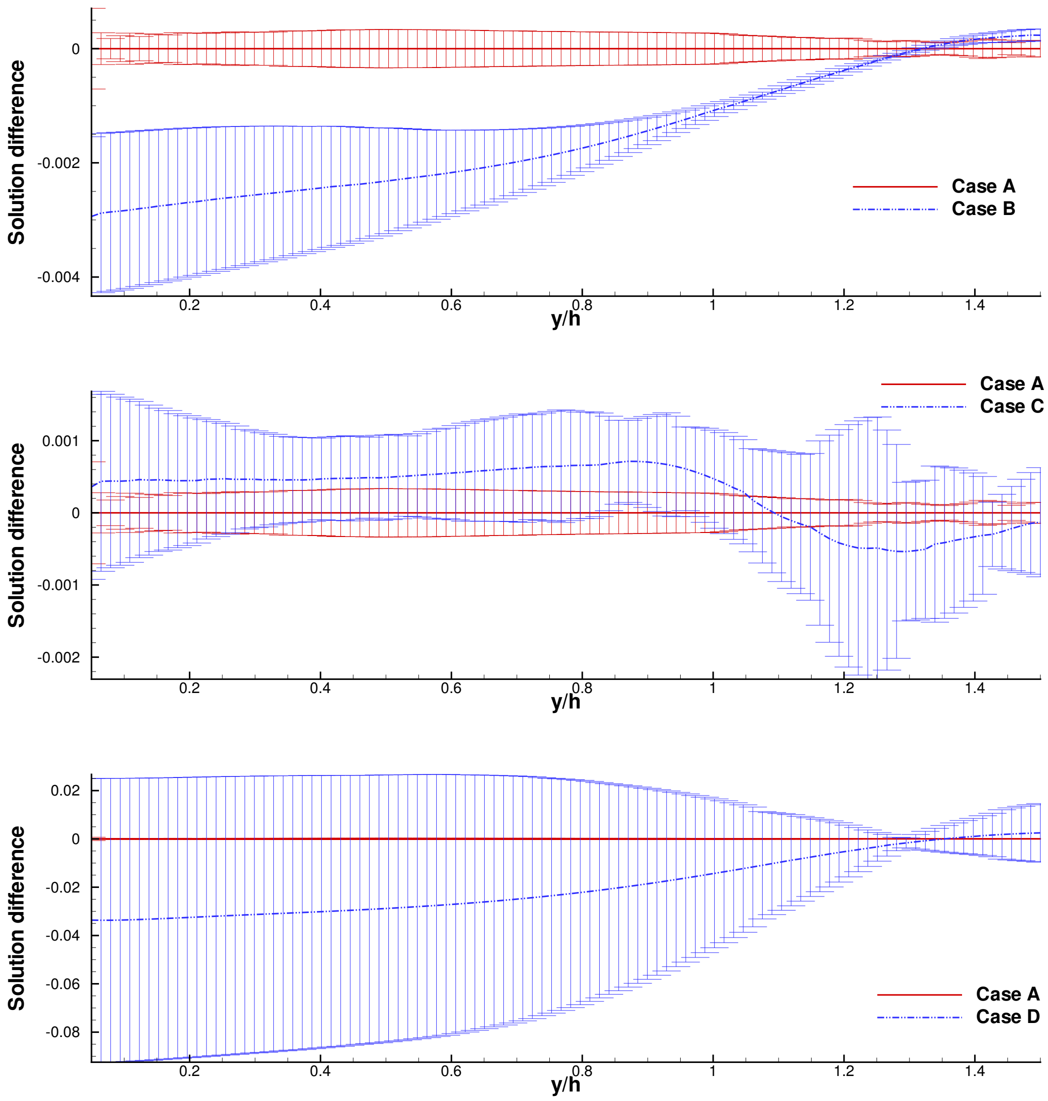

Figure 5: Uncertainty self consistency check at x=7.

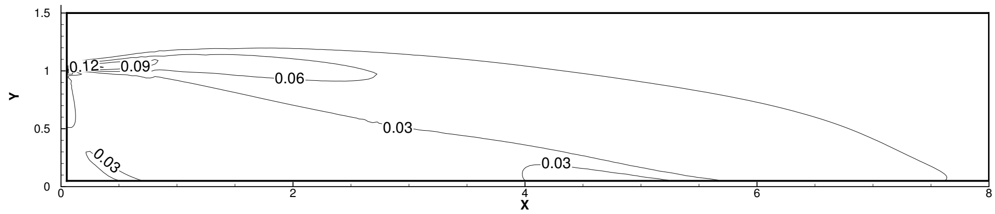

Figure 6: Solution difference between grid A and grid D

unknown. The convergence behaviour of the estimated error norms provides revealing information to the numerical solution. It can also provide an uncertainty estimation for local quantity. For numerical solution with good convergence behaviour, we can expect to obtain a reliable uncertainty estimation for local quantity. When the convergence behaviour is poor, the uncertainty estimation for local quantity may not be correct in some

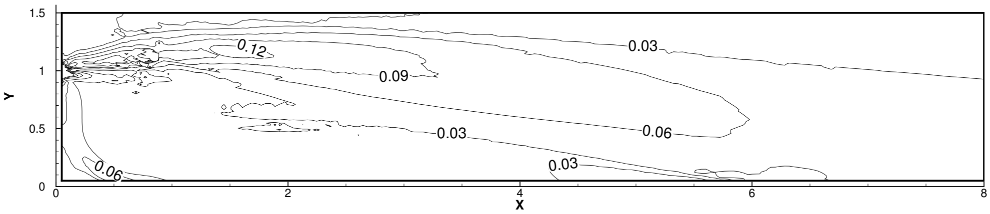

Figure 7: Estimated uncertainty for test case D

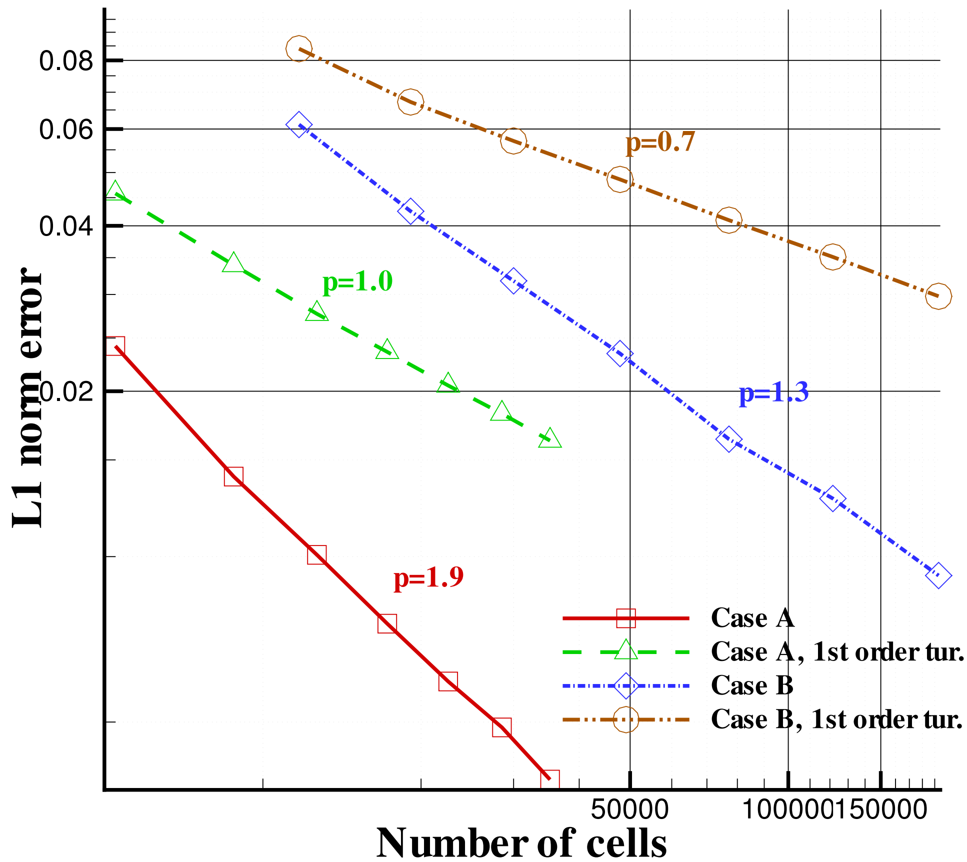

Figure 8: Estimated L1 norm error and order of convergence

region, but the level of the uncertainty is still realistic.

Numerical simulations with different type grid for the backward facing step test case reveal that the order of convergence of a numerical solution depends not only on the numerical discretization scheme, but also the type of grid as well. The solution qualification procedure proposed in this paper is capable to determine the order of convergence of a numerical solution with confidence. Solutions with problematic convergence behavior due to poor grid quality or due to the use of first order discretization scheme for turbulent quantities are clearly identified. With a self adaptive extrapolation procedure, it is possible to give a realistic uncertainty estimation to local quantity without using a too conservative safety factor even when the apparent order of convergence is much lower

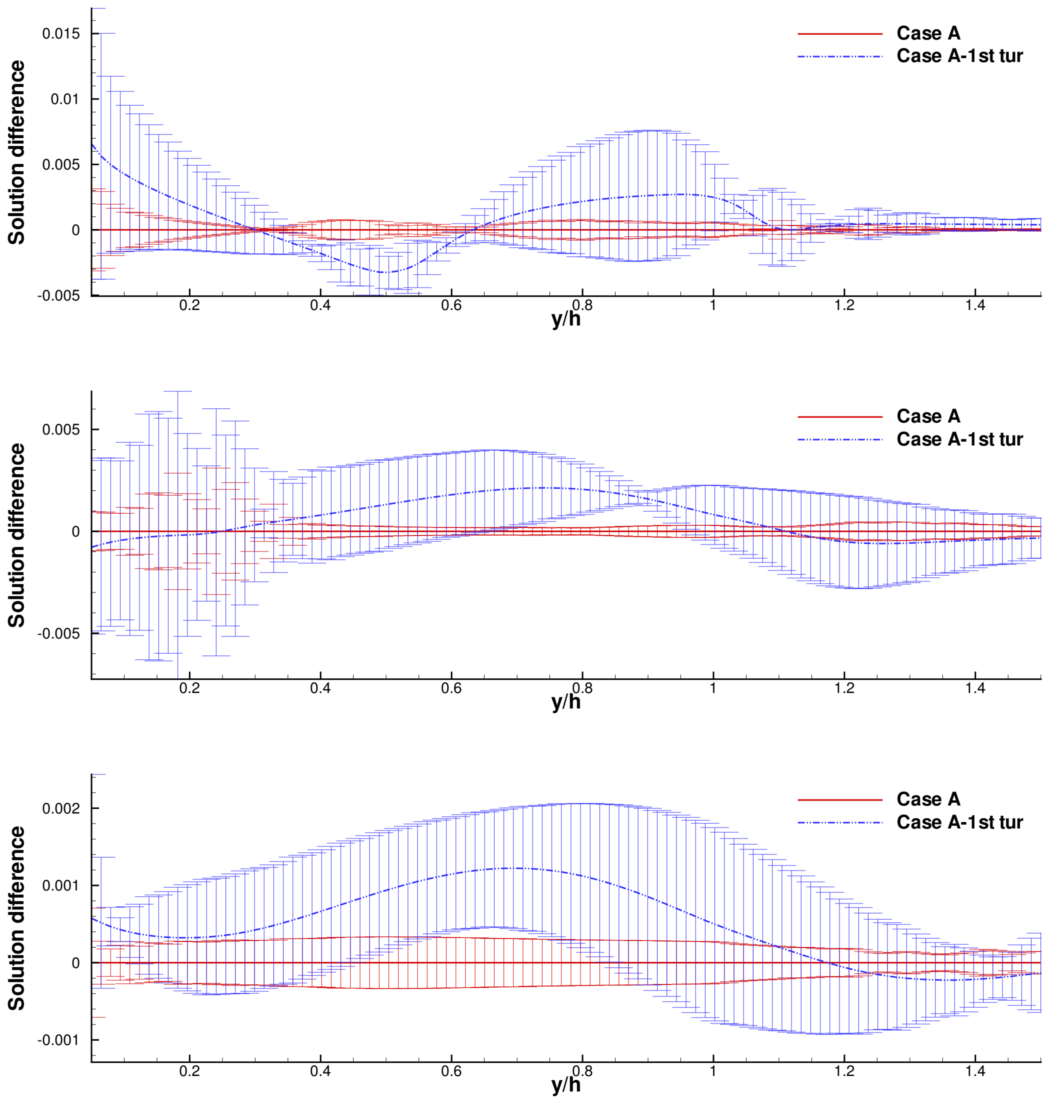

Figure 9: Uncertainty self consistency check for test case A with first order discretization scheme for turbulent transport equations. From up to down, x=1h, x=4h and x=7h

than the expected value.

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