Computation for the Backward Facing Step Test Case with an Open Source Code

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1 Motivation

We have proposed a solution qualification procedure that allows to estimate the order of convergence of a numerical solution. While this procedure can give a correct result when it is applied to a manufactured solution, some unexpected results are observed when it is applied to the backward facing step test case. While a second order accuracy is obtained with the Cartesian grid as expected, the order of accuracy obtained with the multi-block structured grid set is about 1.4. As this multi-block grid is nearly orthogonal, and the grid density is fine enough (up to 200 000 grid nodes), we would also expect a second order convergence. Another unexpected result is that in some region for some quantity, results obtained with these two grid sets do not overlap. We continue the investigation on this issue during the work prepared for this workshop. In order to confirm or infirm these findings, the same exercises are repeated with OpenFoam.

2 Uncertainty Estimation Procedure

The solution qualification procedure was proposed by the author in the second Lisbon workshop [1] and was slightly revised later [2]. For completeness, it is repeated here.

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 done as follows. First, we choose a target region which 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 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. $\mid Diff^0 \mid$ 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

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

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

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

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

$$Err^k = \mid Diff^0 \mid + Diff^k$$

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. [8] 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 on the numerical discretization scheme, but also on the type of grid employed in the computation. Hence, no theoretical order of convergence exists for a numerical solution. The least squares approach proposed by Eça and Hoekstra [4] improves the reliability of the estimation, although it is not always the best choice. We believe that the best extrapolation procedure is a procedure that adjusts itself to the data. In the extrapolation procedure employed in the present study, more than 4 grids are necessary but 5-6 grids are recommended. The 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. An abrupt variation of the apparent order of convergence gives evidence of data scattering. In this case, the 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. An example given in the following section will better illustrate how this self-adaptive approach is applied.

3 Numerical setup in OpenFoam

The steady incompressible solver SimpleFoam (version 1.4-1) has been used for the computation. Gradient is computed with the Gauss linear scheme. Laplacian operator is discretized with the Gauss linear corrected scheme, while the convection operator is handled with a Self-Filtered Central Differencing scheme. Surface normal gradient contains an explicit non-orthogonal correction. Linear scheme is employed for interpolation. The global convergence criterion is set to 1e-10 for all quantities. At each iteration, we try to reduce the residual of each linear system by a factor of 1000 unless the global convergence criterion is satisfied. Bi-conjugate gradient solver is used to solve the transport equation (PBiCG) and the pressure equation (PCG). An under-relaxation factor of 0.25 is applied to all quantities. Non-orthogonal correction in SIMPLE algorithm is not applied since one mesh is orthogonal, and the other is nearly orthogonal. However, one should stress that fully converged solution can not be obtained for all test cases.

4 Application to a backward facing step test case

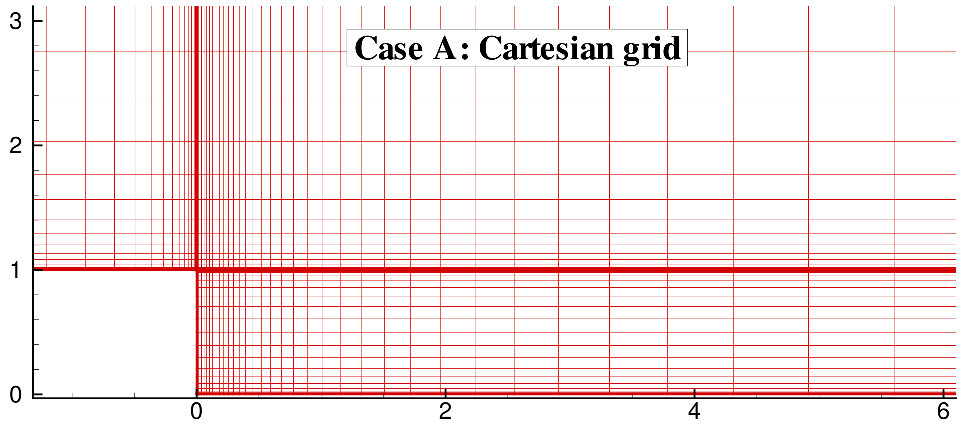
The procedure described above is applied to a backward facing step test case. It is the configuration investigated experimentally by Driver and Seegmiller [3] with zero top-wall angle. The Reynolds number based on the step height, noted h hereafter, and the maximum velocity at the inlet is 50000. The channel height at the inlet is 8h. This test case has been chosen for the two workshops devoted to CFD uncertainty analysis held in Lisbon in 2004 and 2006 [5] [6]. The computational domain started at 4h before the step where inlet profiles for the streamwise velocity component and the turbulent quantities are prescribed by using an initialization program provided by the Lisbon workshop organizers. The Spalart-Allmaras model [7] is employed for turbulence modelization. The computational domain is extended to 40h after the step where zero value is imposed to the pressure, while Neumann boundary conditions are applied to other quantities.

4.1 Mesh for different test cases

Two different grid sets are employed. The first one (test case A) is a Cartesian grid (Figure 1). 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.

4.2 Uncertainty estimation

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



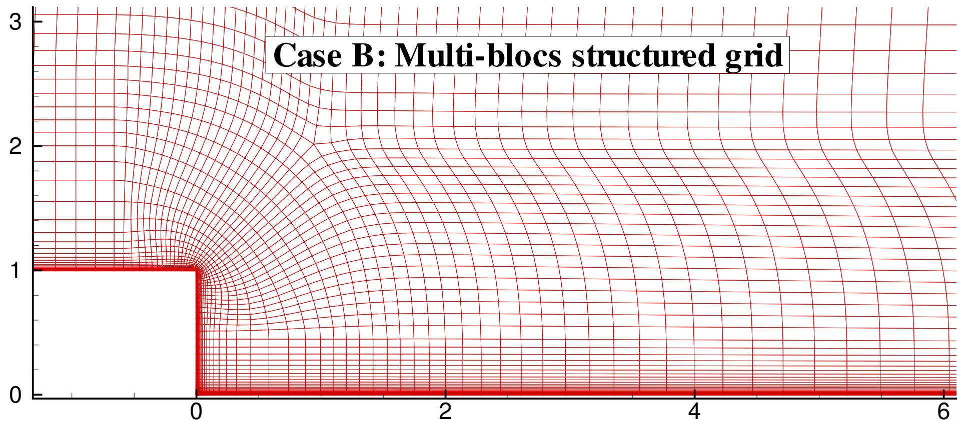


Figure 1: Mesh for different test cases.

Test case A, Cartesian grid

Cartesian grid is employed for this test case. Five grids have been employed for the computation. Number of grid points as well as the solution difference for each grid is displayed in table 1. Results of Richardson extrapolation are shown in table 2. Convergence is observed only for the finest grid triplet. Other results shown in this table are the results obtained with a polynomial approach using a first and a second order term. We retain the result obtained with the finest grid triplet. The estimated L1 norm error for the finest grid is Err^1=0.0232. A safety factor F_s=1.25 is applied. Uncertainty level may be under-estimated with this choice, since using the result of polynomial approach will increase the uncertainty by about a factor of 1.7.

Grid ID	Case A	Case B
Grid 1	0 /28512	0 /121582
Grid 2	3.007E-3/22528	8.057E-3/77118
Grid 3	6.888E-3/17248	2.041E-2/47838
Grid 4	1.058E-2/12672	3.565E-2/30002
Grid 5	1.397E-2/ 8800	5.601E-2/19110

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

Grid set	Case A	Case B
5-4-3	-0.0373/ -	-0.0188/ 1.4
4-3-2	-0.0510/ -	-0.0382/ 1.0
3-2-1	**-0.0232/ 1.0**	-0.0180/ 1.6
5 to 1	-0.0402/ -	**-0.0252 1.3**
4 to 1	-0.0394/ -	-0.0259/ 1.2

Table 2: Richardson extrapolation results for different test cases

Test case B, block-structured grid

Five block-structured grids are used for the computation. Due to data scattering, a least squares approach is the only choice since there is no particular reason to exclude any data. All available solutions are employed for the extrapolation. The estimated L1 norm error for the finest grid is Err^1=0.0252. 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.

Comparison between different test cases

The estimated L1 norm error and the apparent order of convergence for the two cases are shown in figure 2. It can be observed that the two coarsest grids of the Cartesian grid set containing 8800 and 12672 cells, respectively, are too coarse to be included in the uncertainty estimation. The convergence behavior of the multi-block structured grid is good with an order convergence similar to what we obtained with our code using the same grid set, much lower than the expected theoretical second order convergence. As the present approach can give correct estimation to the order of convergence only when a monotonic variation of the solution on different grid is observed, such a low observed order of convergence may due to non-monotonic variation of the solution on different grid in some region. By retaining the points on which monotonic variation is observed in the evaluation, the observed order of convergence with the finest grid triplet is 1.6 and 1.75, respectively, for the Cartesian grid and the multi-block structured grid. These values are closer to the expected second order convergence.

4.3 Uncertainty self consistency check

In this section, the uncertainty estimation is compared for the two 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 locations x=1h, 4h and 7h in figures 3, 4 and 5 respectively. In general, both solutions overlap very well at all locations. The level of numerical uncertainty is about 0.5%, which is acceptable for engineering application. This observation suggests that the use of the finest grid triplet and a safety factor of 1.25 is an appropriate choice.

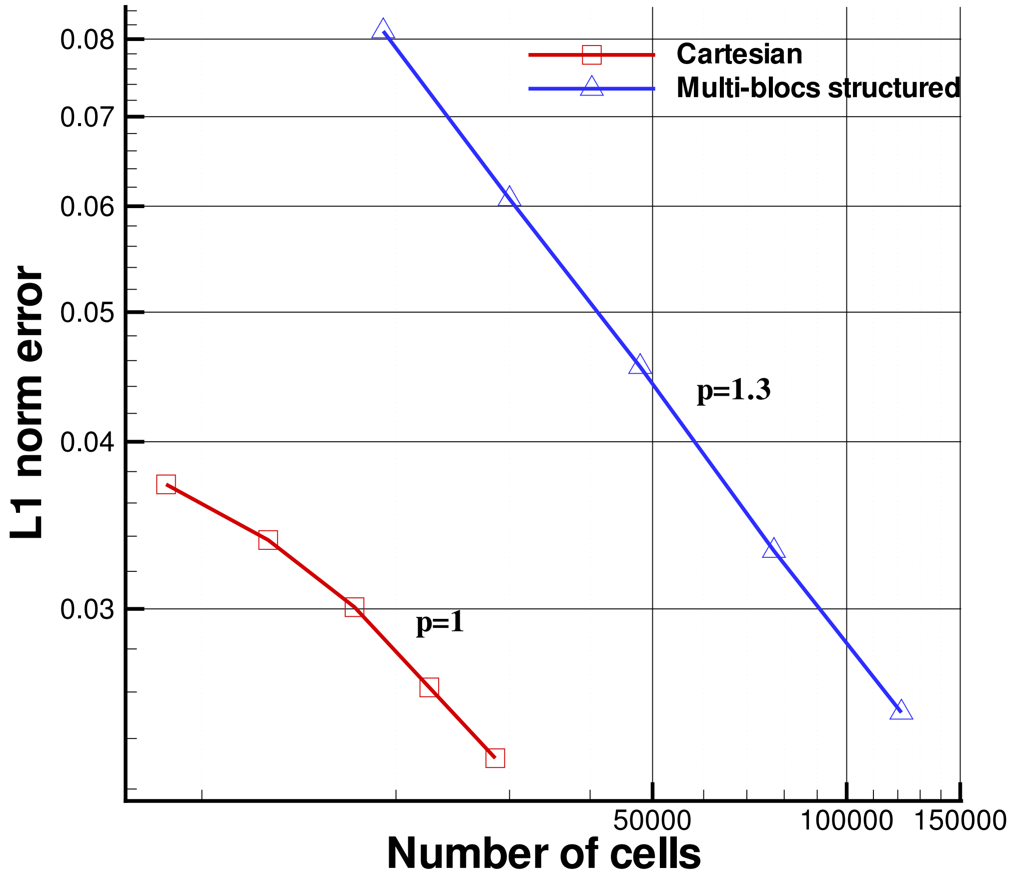


Figure 2: Estimated L1 norm error and order of convergence

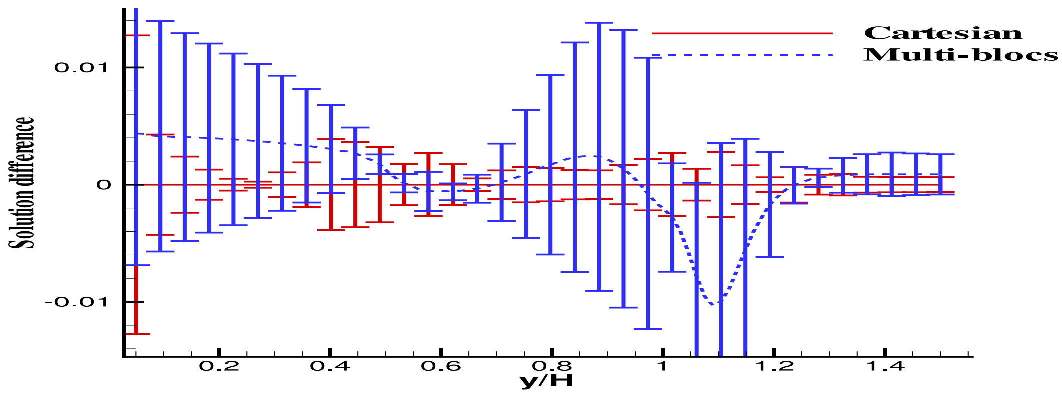


Figure 3: Uncertainty self consistency check at x=1.

5 Conclusion

Results obtained with OpenFoam for the backward facing step test case using two different grid sets are analyzed in this paper. Two results agree well within the uncertainty range. In another paper presented in this workshop [9], the author demonstrates that

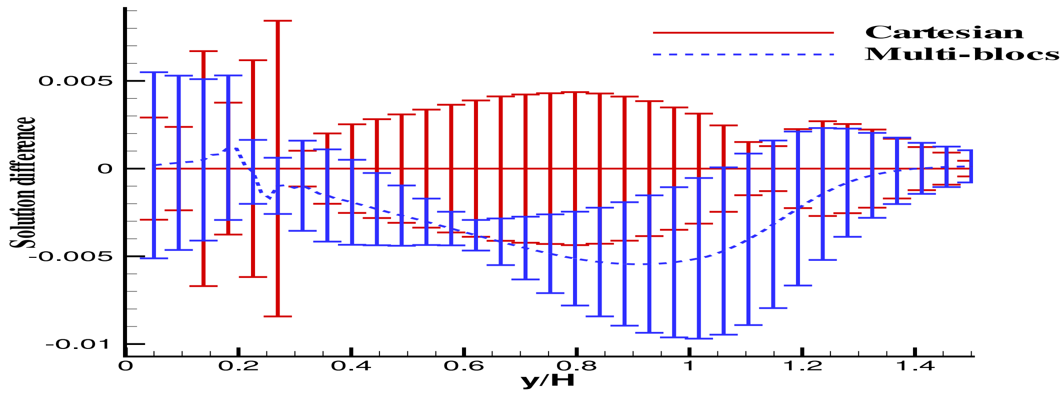


Figure 4: Uncertainty self consistency check at x=4.

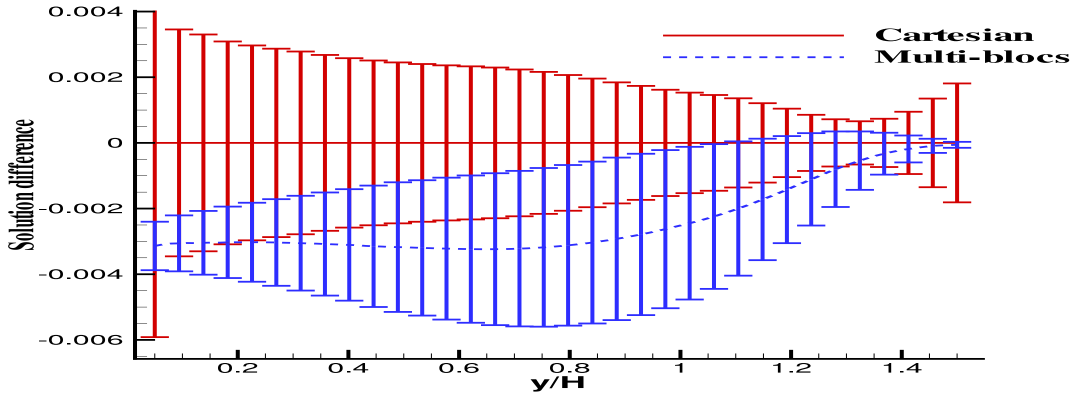


Figure 5: Uncertainty self consistency check at x=7.

the non-overlapping results obtained with the two grid sets employed in this study using our in house code were related to the wall normal distance computation rather than discretization error or coding error. With OpenFoam, the expected second order convergence cannot be obtained, even with the Cartesian grid set, which is very surprising. This observation, which has to be confirmed by other expertised users, suggests that second order convergence with OpenFoam computation is difficult to achieve for engineering application, even in a computation for demonstration purpose. Such kind of convergence is unlikely possible to obtain without a carefully designed grid with appropriate refinement. However, numerical uncertainty on the velocity field can be reduced to about 0.5% with reasonably refined grid, which is satisfactory for engineering application.

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