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A VERIFICATION AND VALIDATION EXERCISE FOR THE FLOW OVER A BACKWARD FACING STEP

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Abstract. *This paper presents Solution Verification and Validation exercises for the flow over a backward facing step. Two completely different flow solvers are applied: ReFRESCO, using a finite-volume discretization of the momentum equations in strong conservation form and a pressure-correction algorithm based on the SIMPLE approach; PARNASSOS, discretizing the non-conservative continuity and momentum equations written in Contravariant form with finite-differences. Two sets of geometrically similar single-block structured grids are selected to perform Solution Verification. A procedure based on a least squares version of the Grid Convergence Index is used to estimate the numerical uncertainty of functional and local flow quantities.*

The iterative error is evaluated for the ReFRESCO calculations by comparing solutions obtained with less demanding convergence criteria to flow fields converged to machine accuracy. As already experienced in similar exercises with PARNASSOS, the iterative error may be 2 to 3 orders of magnitude larger than the L_∞ norm of normalized residuals and/or flow variable changes between consecutive iterations at the last iteration performed. Furthermore, the iterative errors must be two orders of magnitude smaller than the discretization error to have a negligible influence on the determination of the latter.

The present Solution Verification exercise confirms that misleading conclusions may be drawn from numerical simulations without the knowledge of the numerical uncertainty.

An example of the application of the ASME V&V-20 Validation procedure is presented for an horizontal velocity profile downstream of the step. It is clear that the proposed procedure is a step forward compared to the simple graphical comparisons between numerical predictions and experimental data.

1 INTRODUCTION

Many practical problems of fluid dynamics are currently analysed by numerical solution of the mathematical models that simulate the physics of the flows, i.e. by Computational Fluid Dynamics (CFD). In the early years of the development of CFD, it was an achievement already to demonstrate the ability to address the problems using numerical solutions. However, in many current applications of CFD it is no longer enough to produce "a solution". The credibility of the simulations must be established with Verification and Validation[1].

Verification and Validation (V&V) are distinct activities[1]:

- Verification is a purely mathematical exercise consisting of two parts:
  1. Code Verification, intending to demonstrate by error evaluation the correctness of the code that contains the algorithm to solve a given mathematical model.
  2. Solution Verification, attempting to estimate the error/uncertainty of a given numerical solution, for which, in general, the exact solution is unknown.
- Validation is a science/engineering activity meant to show that the selected model is a good representation of the "reality".

This means that Verification deals with numerical (and coding) errors, whereas Validation is related to modelling errors. In the present paper, we will not address Code Verification. An example of Code Verification for a RANS solver (also used in this study) is presented in Eça *et al*[2].

Although there is ample literature on V&V available, as for example the recent books by Roache[3] and by Oberkampf & Roy[4], there are no "all purpose" procedures available for applications involving complex turbulent flows. In fact, the series of Workshops[5,6,7] organized in Lisbon from 2004 to 2008 demonstrated how cumbersome - and at the same time how useful - uncertainty estimation for numerical solutions of the Reynolds-Averaged Navier-Stokes (RANS) equations is. With regard to Validation, the tests performed at the 2008 Workshop[7] with a simplified form[8] of the procedure recently proposed by the ASME V&V-20 committee[9] showed that it is possible to do much better than the common graphical comparisons between experimental data and numerical solutions.

In this paper, we present Solution Verification and Validation exercises for one of the test cases used in the Lisbon Workshops[5,6,7]: the flow over a backward facing step[10]. The aim of the exercise is to compare the outcome of the exercise using solutions obtained with two completely different incompressible flow RANS solvers: ReFRESCO and PARNASSOS. Both codes will be briefly characterised in the sequel.

Numerical uncertainties are estimated with a procedure relying on a least squares version[11] of the Grid Convergence Index[1] and on the data range. Validation is performed with the simplified form of the ASME V&V-20 procedure[8].

The paper is organized in the following way: for the sake of completeness, section 2 presents a brief description of the two flow solvers; the solution verification and validation procedures are presented in section 3 and the selected test case is briefly described in section 4; the solution verification and validation exercises are presented in sections 5 and 6. Finally, section 7 summarizes the main conclusions of this study.

2 FLOW SOLVERS

2.1 ReFRESCO

ReFRESCO is a MARIN spin-off of FreSCo[12], a code which was developed within the VIRTUE EU Project together with TUHH and HSVA. It solves multi-phase (unsteady) incompressible flows with the RANS equations, complemented with turbulence models and volume-fraction transport equations for different phases. The equations are discretized using a finite-volume approach with cell-centered collocated variables. The equations are discretized in strong-conservation form and a pressure-correction equation based on the SIMPLE algorithm (see for example Ferziger & Péric[13]) is used to ensure mass conservation. All equations are segregated in the iterative solution process. The implementation is face-based, which permits grids with elements consisting of an arbitrary number of faces (hexahedrals, tetrahedrals, prisms, pyramids, etc.), and if needed h-refinement (hanging-nodes). The code is parallelized using MPI and sub-domain decomposition, and runs on Linux workstations, clusters and super-computers.

2.2 PARNASSOS

The 2-D version of PARNASSOS solves the Reynolds-averaged Navier Stokes equations for steady, incompressible flows, using eddy-viscosity turbulence models, and is available in finite-difference[14] and finite-volume[15] versions. Here the former version is employed, which means that finite-difference approximations are applied to the continuity and momentum equations written in Contravariant form, which is a weak conservation form. The momentum balance is applied along the directions of the curvilinear coordinate system rather than the directions of the reference coordinate system. The code has a collocated arrangement with the unknowns and the discretization centered at the grid nodes. The linear system of equations formed by the discretized continuity and momentum equations is solved simultaneously. The solution of the turbulence quantities transport equations is uncoupled from solving the continuity and momentum equations.

3 SOLUTION VERIFICATION AND VALIDATION PROCEDURE

3.1 Solution Verification

The aim of Solution Verification is to estimate the numerical uncertainty, U_ϕ, of a solution, ϕ_i for which we do not know the exact solution, ϕ_{exact}. Our goal is to define an interval that contains the exact solution with a 95% confidence,

$$\phi_i - U_\phi \leq \phi_{exact} \leq \phi_i + U_\phi. \tag{1}$$

We will assess the numerical uncertainty of a given flow variable, U_ϕ, as the estimated numerical error estimator multiplied by a factor of safety[3]. Therefore, solution verification requires numerical error estimation.

It is commonly accepted[1] that the numerical error has three components: the round-off error; the iterative error and the discretization error. In problems with smooth solutions, the round-off error becomes negligible with the use of double (15 digits) precision. In principle, the iterative error may be reduced to the level of the round-off error. However, that may be excessively time consuming. Therefore, much less demanding convergence criteria than machine accuracy are generally adopted in practical calculations. However, it has been demonstrated before[16] that the iterative error may be considered negligible only if it is 2 to 3 orders of magnitude smaller than the discretization error. On applying such criterion, one meets two difficulties:

1. The normalized residual norms and/or changes between consecutive iterations obtained in the last iteration performed are not reliable estimators of the iterative error[16,17].

2. The discretization error is not known a priori.

The first problem has been demonstrated for several applications of PARNASSOS[16,17]. In section 5.1, we will show that it also occurs for ReFRESCO, by comparing solutions converged to machine accuracy with intermediate solutions obtained with less demanding convergence criteria.

In the present work, we have reduced the iterative error to machine precision to guarantee that its effect on the numerical error is negligible. The dominant contribution to the numerical uncertainty is then the discretization error.

The basis of the procedure for uncertainty estimation followed in this study is discussed in Eça *et al*[2]. It is constructed for a formally second-order accurate method and it relies preferably on Richardson extrapolation (RE) and the Grid Convergence Index (GCI)[1] to obtain the numerical uncertainty.

The estimate of the discretization error, ϵ, using RE is given by:

$$\epsilon \simeq \delta_{RE} = \phi_i - \phi_o = \alpha h_i^p. \tag{2}$$

ϕ_i stands for any integral of local quantity, ϕ_o is the estimate of the exact solution, α is a constant, h is the typical cell size and p is the observed order of accuracy. The estimation of ϵ requires the determination of ϕ_o, α and p, which in our approach is supposed to be done in the least squares sense using data from at least 4 grids[11], $n_g \geq 4$.

Unfortunately, the determination of p is extremely sensitive to perturbations in the data[11] (even in the least squares sense) and so we can not rely only on δ_{RE} to obtain

ϵ. Furthermore, we can only obtain an error estimate from RE when the convergence is monotonic. Therefore, we have introduced three alternative error estimators (as we mention above, the theoretical order of accuracy is supposed to be $p = 2$):

$$\delta_{RE}^{02} = \phi_i - \phi_o = \alpha_{01} h^2 \ , \tag{3}$$

$$\delta_{RE}^{12} = \phi_i - \phi_o = \alpha_{11} h + \alpha_{12} h^2, \tag{4}$$

and

$$\delta_{\Delta_M} = \frac{\Delta_M}{\left(\dfrac{h_{n_g}}{h_1}\right) - 1}, \tag{5}$$

where Δ_M is the data range

$$\Delta_M = \max\left(|\phi_i - \phi_j|\right) \quad 1 \geq i, j \geq n_g \ . \tag{6}$$

δ_{RE}^{02} and δ_{RE}^{12} are also determined in the least squares sense.

Following the approach of Roache[1], the error estimator is converted to a numerical uncertainty by introducing a safety factor, F_s,

$$U_\phi = F_s \left|\epsilon\right| . \tag{7}$$

Therefore, we have two decisions to make to obtain the uncertainty estimate:

1. Select the most appropriate error estimator.

2. Select the safety factor F_s.

Herein we proceed as follows:

- Determine the apparent convergence condition from the least squares fit:
  - Monotonic convergence for $p > 0$.
  - Oscillatory convergence for $n_{ch} \geq \mathrm{INT}(n_g/3)$ where n_{ch} is the number of triplets with $(\phi_{i+1} - \phi_i)(\phi_i - \phi_{i-1}) < 0$.
  - Otherwise, anomalous behaviour.

- Determine the uncertainty according to the apparent convergence condition:
  - Monotonic convergence:
    * $0.95 \leq p \leq 2.05$:

$$U_\phi = 1.25\delta_{RE} + U_s. \tag{8}$$

    * $p \leq 0.95$:

$$U_\phi = \min\left(1.25\delta_{RE} + U_s, 3\delta_{RE}^{12} + U_s^{12}\right). \tag{9}$$

  * $p \geq 2.05$:

$$U_\phi = \max\left(1.25\delta_{RE} + U_s, 3\delta_{RE}^{02} + U_s^{02}\right). \tag{10}$$

- Oscillatory convergence:

$$U_\phi = 3\delta_{\Delta_M}. \tag{11}$$

- Anomalous behaviour:

$$U_\phi = \min\left(3\delta_{\Delta_M}, 3\delta_{RE}^{12} + U_s^{12}\right). \tag{12}$$

U_s, U_s^{02} and U_s^{12} are the standard deviations of the least squares fits and the safety factor, already included in the previous equations, follows the basic options of the GCI[1]: $F_s = 1.25$ if p is reasonable ($0.95 \leq p \leq 2.05$) and $F_s = 3$ otherwise.

3.2 Validation procedure

The aim of Validation is to estimate the modelling error of a given mathematical model in relation to a given set of experimental data (physical model). It involves numerical, experimental and parameter uncertainties. Thus the mathematical model can be validated against that particular experiment. If the validation is successful one cannot say that the code is validated, only that the model is valid for the flow problem at hand.

A well-documented procedure has been proposed recently by the ASME[9,8]. It compares two quantities:

- The validation uncertainty, U_{val},

$$U_{val} = \sqrt{U_{num}^2 + U_{input}^2 + U_D^2}.$$

- The validation comparison error, E,

$$E = S - D.$$

U_{num} is the numerical uncertainty for the quantity ϕ chosen (U_ϕ from the previous section), U_{input} is the parameter uncertainty, (due to possible uncertainties in the fluid properties, flow geometry and/or boundary conditions), and U_D is the experimental uncertainty. S is the numerical prediction (ϕ_i in the previous section) and D the experimental value.

The goal of the procedure is to determine the interval that contains the modelling error, δ_{model}, with 95% confidence: $[E - U_{val}, E + U_{val}]$. The outcome of the exercise is decided from the comparison of $|E|$ with U_{val}:

- If $|E| >> U_{val}$ the comparison error is probably dominated by the modelling error, which indicates that the model must be improved.

- For $|E| < U_{val}$, δ_{model} is within the "noise level" imposed by the numerical, experimental and parameter uncertainties. It can mean two things: if E is considered sufficiently small, the model and its solution are validated (with U_{val} precision) against the given experiment; else the quality of the numerical solution and/or the experiment should be improved before conclusions can be drawn about the adequacy of the mathematical model.

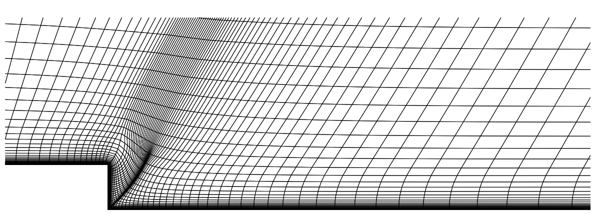
4 TEST CASE

The selected test case is the flow over a backward facing step[10] that has been used as one of the test cases of the Lisbon Workshops[5,6,7]. The experimental data and their uncertainty are taken from Driver *et al*[10] and Jovic & Driver[18]. All the calculations performed in this study were performed using the one-equation eddy-viscosity model proposed by Spalart & Allmaras[19].

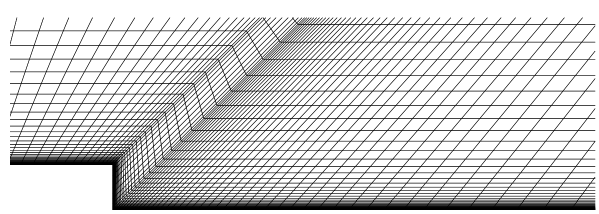
4.1 Computational domain and boundary conditions

The computational domain of the flow around a backward facing step is bounded by two walls and two x constant planes, $-4H$ upstream and $40H$ downstream of the step, where H is the step height. The Reynolds number based on the step height and the velocity of the incoming flow, U_{ref}, is 5×10^5.

In the present calculations, we have specified all the required flow quantities at the inlet, with the exception of the pressure coefficient, using the profiles available from the Lisbon Workshops[5,6,7]. The pressure coefficient is linearly extrapolated from the interior of the domain. At the walls, the no-slip and impermeability conditions are applied, which leads to $u_x = u_y = 0$. The dependent variable of the turbulence model $\tilde{\nu}$, an undamped eddy-viscosity, is set equal to 0. At the outlet boundary, u_x, u_y and $\tilde{\nu}$ are linearly extrapolated from the interior of the domain. The pressure coefficient is set equal to zero.



Set A



Set B

Figure 1: Illustration of the two grids sets for the calculation of the flow over a backward facing step.

4.2 Grid sets

We have selected two sets of 11 single-block, structured, geometrically similar grids, A and B, to perform the calculations of the flow over a backward facing step. Set A contains non-orthogonal curvilinear grids with the same number of nodes in both directions. At the walls, the grids are orthogonal. Set B has straight lines connecting the bottom and top walls and the same number of nodes in both directions. In both sets, the coarsest grids have 101×101 nodes (10^4 cells) and the finest grids 401×401 nodes (1.6×10^5 cells) covering a grid refinement ratio of 4. The grids in the vicinity of the step are illustrated in figure 1. Under the restrictions of a single-block structured grid, the grid properties are not as good as they might be for unstructured or for multi-block structured grids.

5 VERIFICATION EXERCISE

As we mentioned above, all the calculations were performed with 15 digits precision and the iterative error was reduced to machine accuracy. This ensures that round-off and iterative errors are negligible in the determination of the numerical uncertainty. Before we present the results of the estimated discretization uncertainties, we illustrate the need to use reliable iterative error estimators when the convergence criteria are substantially less demanding than machine accuracy.

5.1 Iterative error

Practical calculations of complex turbulent flows are seldom being converged to machine accuracy. It is then often supposed that the normalized residuals and/or changes between consecutive iterations obtained in the last iteration, are a proper measure for the iterative error. However, as illustrated for the 2-D and 3-D[15,20] versions of PARNASSOS[16,17], these quantities are not reliable iterative error estimators.

Unlike the discretization error that requires the knowledge of the exact solution, a good estimate of the iterative error may be obtained from a solution converged to machine accuracy. In this paper, we present for ReFRESCO a similar study as reported earlier for PARNASSOS[16,17].

Calculations were performed for the grids of set A with different convergence criteria based on the largest value of the L_∞ norm of the normalized residuals of the x and y momentum equations, pressure correction and $\tilde{\nu}$ transport equation. The residuals were made non-dimensional using reference variables and the main diagonal of the algebraic systems of equations. This means that the normalized residuals are equivalent to the non-dimensional variable changes for a simple Jacobi iteration.

Four different levels of the convergence tolerance, e_t, were tested: 10^{-3}, 10^{-5}, 10^{-7} and 10^{-13}. The latter e_t value corresponds to machine accuracy. At the start of the iterative computation process uniform values for all variables were set, with the exception of the imposed boundary conditions.

As an example of the iterative convergence of ReFRESCO, figure 2 presents the L_∞ norms of the normalized residuals and of the changes between consecutive iterations as a function of the iteration counter for the 200×200 cells grid. The two quantities show equivalent convergence histories with all flow variables converging with similar rates to

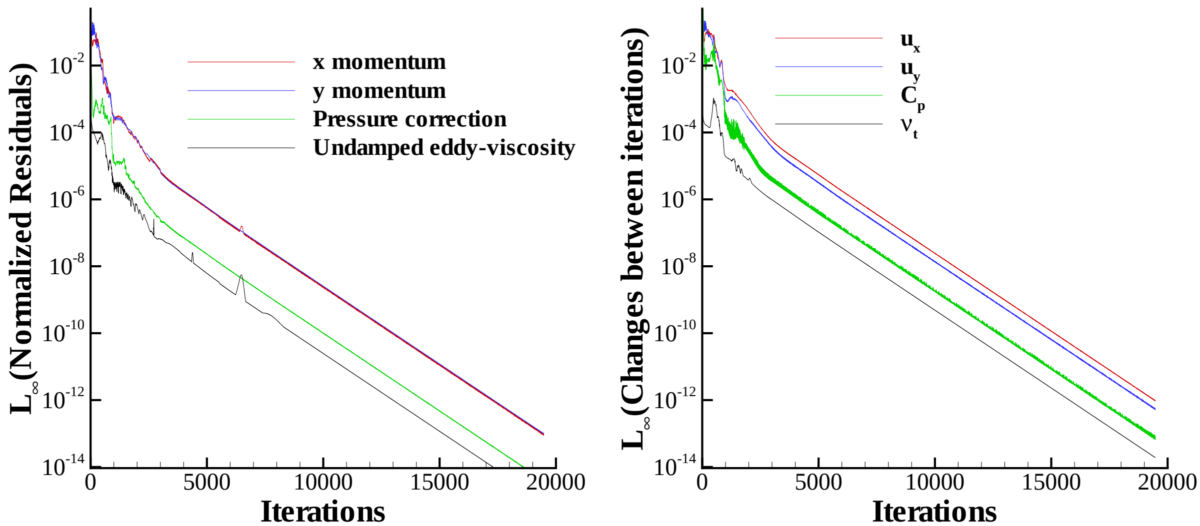


Figure 2: L_∞ norms of the normalized residuals and of the changes between consecutive sweeps as a function of the iteration counter for the 200×200 cells grid.

machine accuracy. The number of iterations required to satisfy $e_t = 10^{-13}$ is roughly four times larger than the number of iterations that satisfies a convergence criteria of $e_t = 10^{-7}$.

For the three highest values of e_t, we have computed the L_∞, L_1 and L_2 norms of the iterative errors (the difference to the solution converged to machine accuracy) of the non-dimensional mean flow variables u_x, u_y and C_p (ρU^2_{ref} is the reference pressure). The results for u_x (one of the variables that drives convergence) are illustrated in figure 3 as a function of the grid refinement ratio, h_i/h_1, which in this case is simply defined by

$$\frac{h_i}{h_1} = \sqrt{\frac{(N_{cells})_1}{(N_{cells})_i}} \; . \tag{13}$$

The plots in figure 3 present the three error norms of the horizontal velocity component in the 11 grids of set A and the iterative error distribution for the 200×200 cells grid for $e_t = 10^{-3}$, $e_t = 10^{-5}$ and $e_t = 10^{-7}$. The data confirm all the trends observed with PARNASSOS[16,17]:

- All error norms of the iterative error are consistently larger than the L_∞ norm of the normalized residuals in the last iteration performed. For the L_∞ norm of the iterative error, they differ more than 3 orders of magnitude!

- As expected, for the same convergence criterion, the iterative error increases with the grid refinement due to the decrease of the iterative convergence rate (no multigrid techniques were applied in this study).

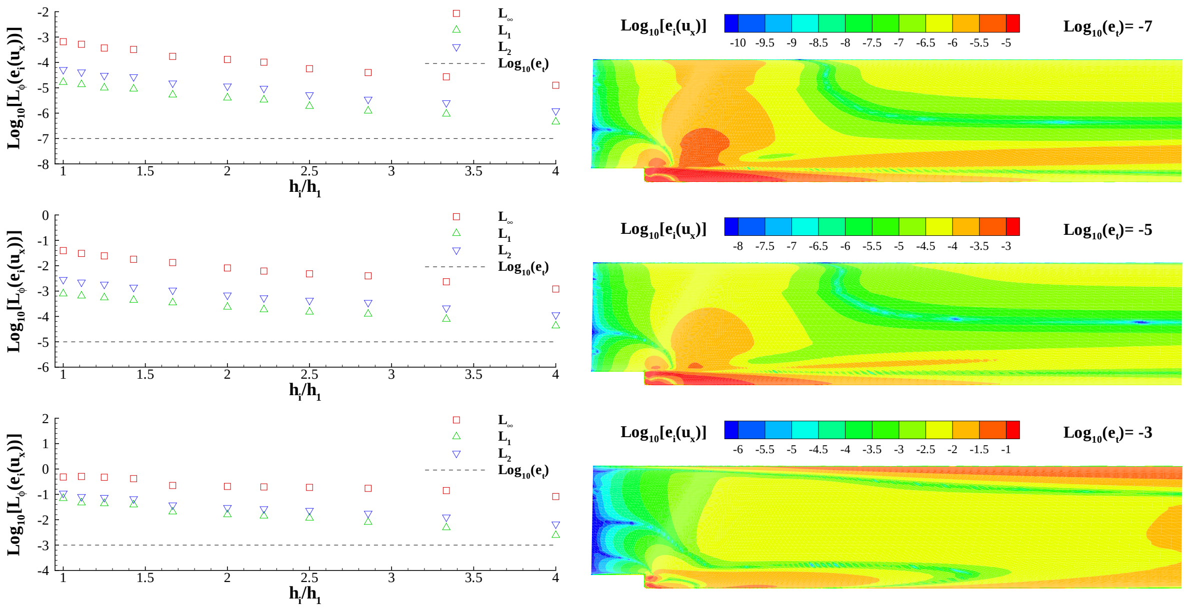


Figure 3: (left) Iterative errors for the horizontal velocity component, u_x, in the grids of set A. Convergence criteria, e_t, based on the L_∞ norm of the normalized residuals. (right) Iterative error field for 200×200 cells grid, $h_i = 2h_1$.

- The iterative error distributions obtained for the three convergence criteria show several similarities. In a large percentage of the field, the iterative error is larger than e_t. It is clear that the solution obtained for $e_t = 10^{-3}$ (which is suggested as the default convergence criterion in some commercial codes) has an unacceptable iterative error.

In the next section we will present an example of the consequences of insufficient iterative convergence on the estimation of the discretization error/uncertainty.

5.2 Discretization error/uncertainty

Several functional and local flow quantities have been proposed for the 2008 Lisbon Workshop[7]. In the present paper, we have selected some of these quantities to compare the results obtained with ReFRESCO and PARNASSOS. In both codes, the nominal order of accuracy of the discretization procedure is 2, with the exception of the convective terms of the $\tilde{\nu}$ transport equation that are approximated with first-order upwind (a "standard" option in the so-called "practical" calculations).

For each of the flow variables presented below, we have estimated the uncertainty of the finest grid solution based on the data of the six finest grids of each set and the uncertainty of the $h_i = 2h_1$ prediction using the data of the six coarsest grids.

We emphasize that the present comparison is not a Code Verification (which would require an exact solution) exercise. The aim of this study is to give one more example of the misleading conclusions that may be drawn from numerical predictions without the knowledge of their numerical uncertainty.

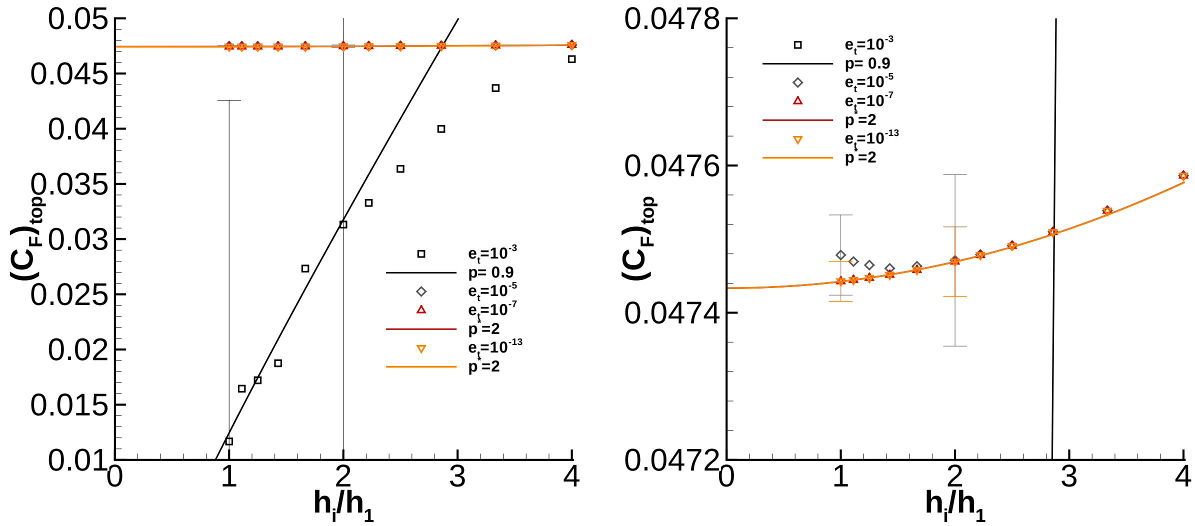


Figure 4: Convergence with the grid refinement of the friction resistance of the top wall resistance coefficient, $(C_F)_{top}$, for different levels of the convergence criteria (right figure is detail of left figure).

5.2.1 Influence of the iterative error on the estimation of the discretization error/uncertainty

Two flow quantities have been selected to illustrate the effect of the iterative error on the estimation of the discretization error/uncertainty: the friction resistance coefficient of the top wall, $(C_F)_{top}$, and the non-dimensional horizontal velocity component, u_x at $x = H$, $y = 0.1H$. Figures 4 and 5 present results of these two quantities as a function of the grid refinement ratio, h_i/h_1, for $e_t = 10^{-3}$, $e_t = 10^{-5}$, $e_t = 10^{-7}$ and $e_t = 10^{-13}$. The data refer to the ReFRESCO calculations in grid set A.

Table 1 summarizes the iterative errors, e_i, of the three solutions with the highest values of e_t (obtained from the difference to the solution converged to machine accuracy) and the estimated discretization uncertainty, U, based on the data obtained with $e_t = 10^{-13}$.

Particularly for $e_t = 10^{-3}$ on fine grids the results are dramatic. It is clear that it is impossible to make a reliable estimation of the discretization error for a convergence criterion of $e_t = 10^{-3}$. For the other two convergence criteria, the results confirm the experience reported in previous studies[16]: the iterative error must be two orders of magnitude smaller than the discretization error to have a negligible effect in the determination of the latter.

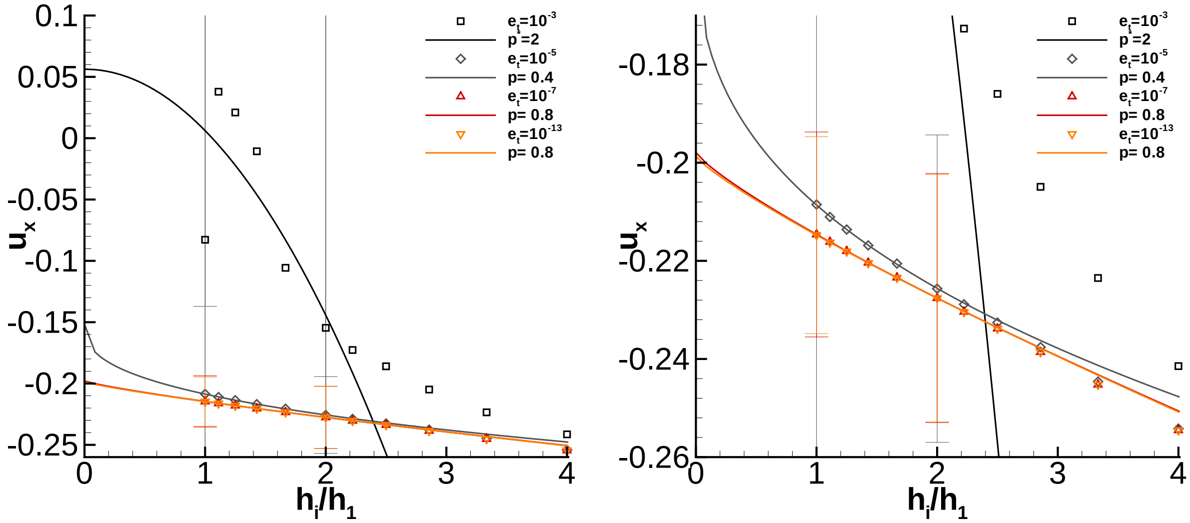


Figure 5: Convergence with the grid refinement of the horizontal velocity component, u_x, at $x = H, y = 0.1H$ for different levels of the convergence (right figure is detail of left figure).

Flow Variable	Iterative error, e_i			Discretization
	$e_t = 10^{-3}$	$e_t = 10^{-5}$	$e_t = 10^{-7}$	Uncertainty, U, for $e_t = 10^{-13}$
$(C_F)_{top}$	3.6×10^{-2}	3.6×10^{-5}	1.1×10^{-7}	2.7×10^{-5}
u_x	1.3×10^{-1}	6.2×10^{-3}	1.4×10^{-4}	2.0×10^{-2}

Table 1: Iterative errors, e_i, for the friction resistance of the top wall resistance coefficient, $(C_F)_{top}$, and the horizontal velocity component, u_x, at $x = H, y = 0.1H$. Estimated discretization uncertainty, U, for the solution converged to machine accuracy.

5.2.2 Functional flow quantities

Figure 6 presents the convergence with grid refinement of the friction resistance of the top and bottom wall, $(C_F)_{top}$ and $(C_F)_{bottom}$ and the pressure resistance coefficient, $(C_D)_{bottom}$, of the vertical wall of the step. The plots contain the data obtained with ReFRESCO and PARNASSOS in the two grid sets.

- All the estimated uncertainties are consistent, i.e. there is overlap between the error bars of the two codes in the two grid sets.
- Some of the estimated uncertainties are surprisingly large. However, these are a consequence of the inability to establish the observed order of accuracy, p, or due to an unexpected small value of p. This is not a surprising result[7], because even with the present grid density it is almost sure that most of the data are outside the "asymptotic range".
- As experienced in many other exercises, the convergence of different flow quantities

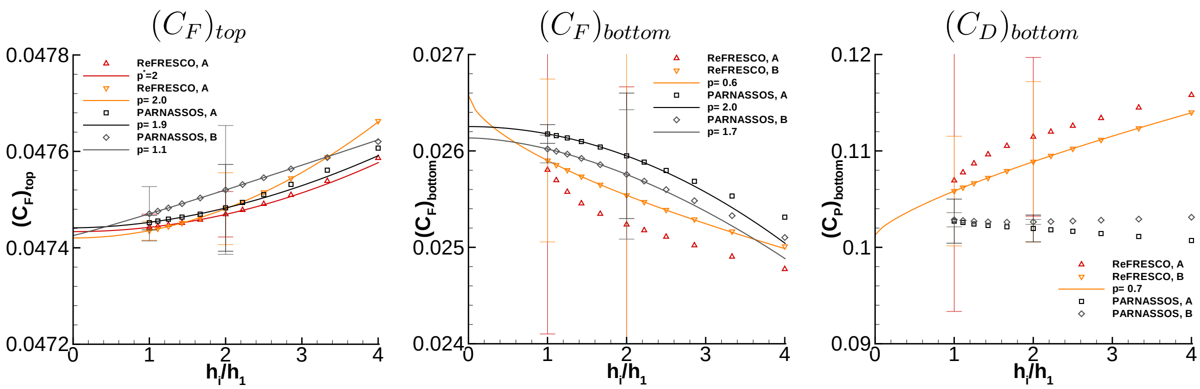


Figure 6: Convergence with the grid refinement of the the friction resistance of the top and bottom wall, $(C_F)_{top}$ and $(C_F)_{bottom}$ and the pressure resistance coefficient, $(C_D)_{bottom}$, of the vertical wall of the step.

does not show similar trends (independently of the selected code).

- Also the two codes show distinct behaviour in grid convergence. They should approach the same solution for $h \rightarrow 0$, but their different numerical properties cause that for finite h their solutions may differ.
- Only $(C_F)_{top}$ exhibits the expected trend of an uncertainty for h_1 smaller than the value obtained for $h_i = 2h_1$. However, $(C_F)_{top}$ is the only variable that gave consistent observed orders of accuracy.
- Fair judgement of the quality of numerical solutions based on single-grid studies without any knowledge of the numerical uncertainty is almost impossible.

5.2.3 Local flow quantities

The convergence of local flow quantities is illustrated at two of the selected locations of the Lisbon Workshops[5,6,7]: $x = H, y = 0.1H$ and $x = 4H, y = 0.1H$. Figure 7 presents the behaviour with grid refinement of the non-dimensional horizontal and vertical velocity components, u_x and u_y and of the non-dimensional eddy-viscosity (reference value equal to $U_{ref}H$), ν_t, for the four sets of calculations.

The results confirm all the difficulties experienced before in uncertainty estimation for RANS solutions.

- The convergence properties depend on the selected code, grid set, location and flow variable. We have left out the turbulence model because all the data was obtained with the same model.
- Although unpleasantly large in some cases, the estimated error bars are still consistent with a single exception: u_x at $x = 4H, y = 0.1H$. However, the two "failures"

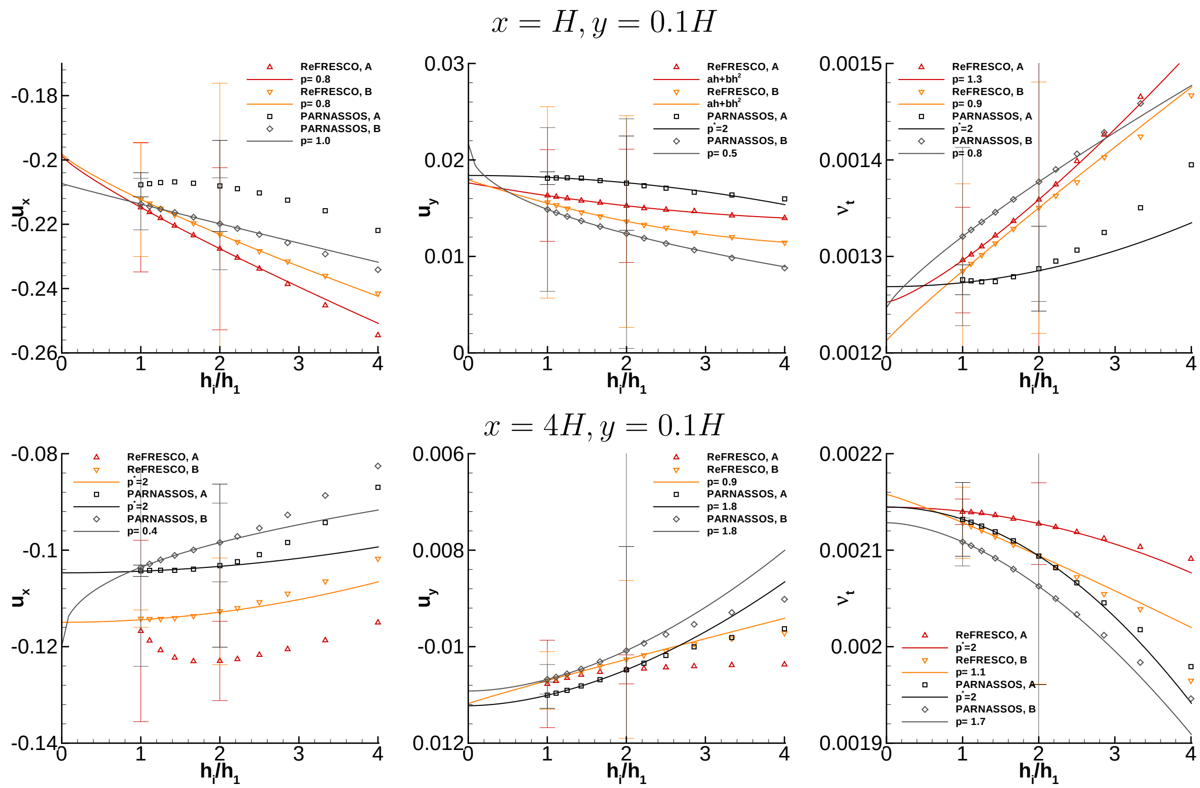


Figure 7: Convergence with the grid refinement of the non-dimensional horizontal and vertical velocity components, u_x and u_y and eddy-viscosity, ν_t, at $x = H, y = 0.1H$ and $x = 4H, y = 0.1H$.

(one for each code and each grid set) are obtained from data that is "suspiciously" similar in the last six grids of the sets.

- The variety of values obtained for the observed order of accuracy is not encouraging for "practical procedures" that rely on it.

As for the functional flow quantities, the data plotted in figure 7 confirm that the numerical uncertainty is fundamental information for the assessment of the quality of any numerical prediction. Furthermore, as demonstrated in the previous sections, the concern about numerical errors is not restricted to discretization errors.

6 VALIDATION EXERCISE

As for the solution verification test, there were several flow quantities proposed for the Validation exercise of the 2008 Lisbon Workshop[7]. In the present study, we will restrict ourselves to the horizontal velocity profile at one step height downstream of the step corner $x = H$. It must be mentioned that this simple exercise requires interpolation of the computed flow fields to the measured locations. A careful choice of the interpolation procedure is required to avoid numerical solutions contaminated by the interpolation error.

The discussion of such procedures is out the scope of this paper. However, it is obviously easier to perform such interpolations in a structured grid than in an unstructured grid.

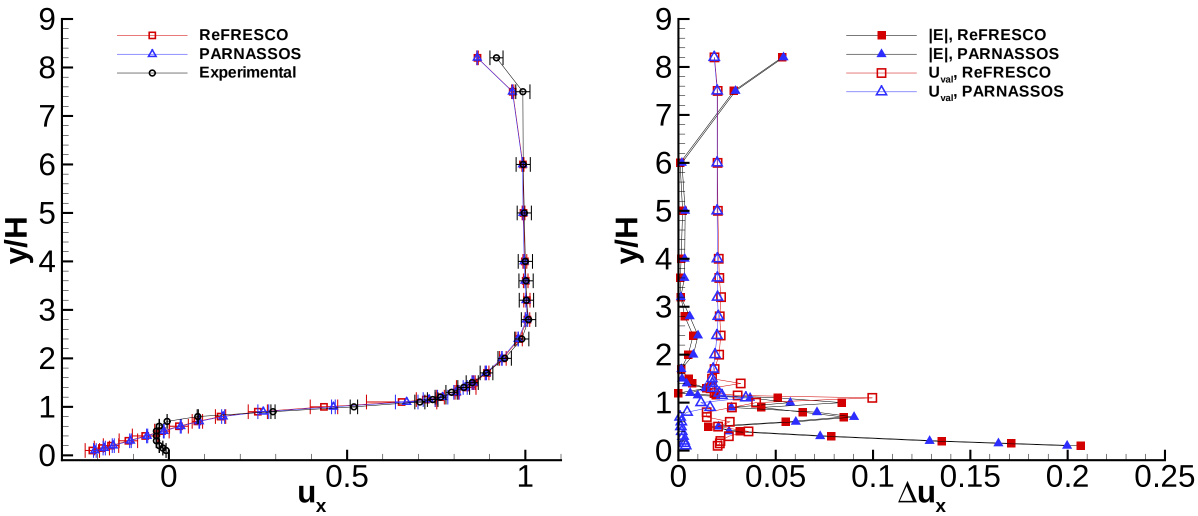


Figure 8: Horizontal velocity component, x, profile at $x = H$. Comparison of predictions and experimental data.

Figure 8 presents the comparison of the ReFRESCO and PARNASSOS predictions with the experimental data[10]. The figure includes two plots: a conventional comparison including the error bars of numerical predictions and experimental measurements (which is not really conventional); the comparison of validation uncertainty, U_{val}, with the comparison error, $|E|$. Both options present useful information:

- Although the estimated numerical uncertainties are not the same for both codes, the outcome of the validation exercise is similar for the two codes.

- In the near-bottom (flow reversal) region it is clear that there is a mismatch between the experimental data and the predictions. The comparison error, $|E|$, is above the validation uncertainty, U_{val} showing that there is a modelling deficiency.

- For $1.5H < y < 6H$, $|E|$ is clearly smaller than U_{val}. This means the numerical solution is "validated". However, the level of the validation uncertainty is $U_{val} \simeq 0.02$. If such level is considered too large, the reduction of U_{val} is mainly dependent on the experimental uncertainty. Therefore, it is the experimental data that require improvement!

- Close to the top wall ($y > 6H$), $|E|$ is (again) larger than U_{val}. However, in this region the results are independent of the selected turbulence model[7]. This suggests that the problem is originated by the specification of the inlet boundary conditions.

Due to the absence of experimental information[10], it was assumed that the top wall boundary-layer was equal to the measured bottom wall boundary-layer[7].

7 CONCLUSIONS

The present paper has presented a Solution Verification and Validation exercise for the flow over a backward facing step. The study was performed with two completely different RANS solvers complemented by the one-equation eddy-viscosity model of Spalart & Allmaras. ReFRESCO uses a finite-volume discretization of the momentum equations written in strong conservation form for volumes of arbitrary shape; continuity is solved indirectly with a pressure-correction equation based on the SIMPLE algorithm. PARNASSOS solves the continuity and momentum equations written in Contravariant form as a coupled set, using finite-difference approximations.

Two sets of geometrically similar single-block structured grids were selected to perform Solution Verification. A procedure based on a least squares version of the Grid Convergence Index was used to estimate the numerical uncertainty of functional and local flow quantities.

The iterative error was evaluated for the ReFRESCO calculations (similar exercises have been performed previously for PARNASSOS) by comparing solutions obtained with less demanding convergence criteria to flow fields converged to machine accuracy. The results confirmed the main trends observed in previous studies:

- Norms of normalized residuals and changes between consecutive iterations are not reliable error estimators.
- The iterative error may be 2 to 3 orders of magnitude larger than the L_∞ norm of normalized residuals and/or flow variable changes between consecutive iterations at the last iteration performed.
- The iterative errors must be two orders of magnitude smaller than the discretization error to have a negligible influence in its determination.

For the selected flow quantities, consistent error bars were obtained for the finest grids solutions obtained with ReFRESCO and PARNASSOS. However, in several cases, the estimated uncertainties are unpleasantly large. Bearing in mind the properties of the selected grid sets and the reported experiences with RANS solvers in similar exercises this is not really a surprising result. Furthermore, the results obtained show convergence properties that depend on the code, grid set, flow variable and selected location (the turbulence model is not in the list because we have used only one). There are several examples in the data that show large mismatches between the predictions of the two codes for a given grid refinement level. However, these are only a consequence of different grid convergence properties of the codes. Therefore, the present exercise confirms that misleading conclusions may easily be drawn from numerical simulations without the knowledge of the numerical uncertainty.

An example of the application of the ASME V&V-20 Validation procedure is presented for an horizontal velocity profile downstream of the step. It is clear that the proposed procedure is a step forward compared to the simple graphical comparisons between numerical predictions and experimental data. It clearly points out where improvements are required in the mathematical model and where better experimental data are needed to achieve validation.

REFERENCES

[1] Roache, P.J., Verification and Validation in Computational Science and Engineering, *Hermosa Publishers*, New Mexico, 1998.

[2] Eça, L., Vaz, G., Hoekstra, M., Code Verification, Solution Verification and Validation in RANS Solvers, *In Proceedings of ASME 29th International Conference OMAE2010*, Shanghai, China, June 6-11, 2010.

[3] Roache, P.J., Fundamentals of Verification and Validation, *Hermosa Publishers*, New Mexico, 2009.

[4] Oberkampf, W.L., Roy, C. J., Verification and Validation in Scientific Computing, to be published October 2010, *Cambridge University Press*, Cambridge 2010.

[5] *Proceedings of the Workshop on CFD Uncertainty Analysis*, Eça, L., Hoekstra, M. Eds., Lisbon, October 2004.
http://www.maretec.ist.utl.pt/html_files/CFD_workshops/Workshop_2004.htm

[6] *Proceedings of the Workshop on CFD Uncertainty Analysis*, Eça, L., Hoekstra, M. Eds., Lisbon, October 2006.
http://www.maretec.ist.utl.pt/html_files/CFD_workshops/Workshop_2006.htm

[7] *Proceedings of the Workshop on CFD Uncertainty Analysis*, Eça, L., Hoekstra, M. Eds., Lisbon, October 2008.
http://www.maretec.ist.utl.pt/html_files/CFD_workshops/Workshop_2008.htm

[8] Validation Procedure for 3rd Workshop on CFD Uncertainty Analysis, *Proceedings of the 3rd Workshop on CFD Uncertainty Analysis*, Instituto Superior Técnico, Lisbon, October 2008.

[9] ASME Guide on Verification and Validation in Computational Fluid Dynamics and Heat Transfer, *ASME Committee PTC-61, 2008*, ANSI Standard V&V-20, 2009.

[10] Driver, D., Seegmiller, M., Lee, H., Features of a Reattaching Turbulent Shear Layer in Divergent Channel Flow, *AIAA Journal*, Vol. 23, N^o 2, February 1985, pp. 163-171.

[11] Eça, L., Hoekstra, M., An Evaluation of Verification Procedures for CFD Applications, *24th Symposium on Naval Hydrodynamics*, Fukuoka, Japan, July 2002.

[12] Vaz, G., Jaouen, F., and Hoekstra, M., Free-Surface Viscous Flow Computations. Validation of URANS Code FreSCo. *In Proceedings of ASME 28th International Conference OMAE2009*, Honolulu, Hawaii, USA, June 2009.

[13] Ferziger, J. H., Perić M., Computational Methods for Fluid Dynamics, *Springer-Verlag*, Berlin Heidelberg, 1997.

[14] Jacob, J., Eça, L. , 2-D Incompressible Steady Flow Calculations with a Fully Coupled Method, *VI Congresso Nacional de Mecânica Aplicada e Computacional*, Aveiro, Portugal, April 2000.

[15] Hoekstra M., Numerical Simulation of Ship Stern Flows with a Space-marching Navier-Stokes Method, *PhD Thesis*, Delft 1999.

[16] Eça, L., Hoekstra, M., Evaluation of Numerical Error estimation based on Grid Refinement Studies with the Method of the Manufactured Solutions, *Computers and Fluids*, Volume 38, Issue 8, September 2009, p.p. 1580-1591.

[17] Eça, L., Hoekstra, M., On the Influence of the Iterative Error in the Numerical Uncertainty of Ship Viscous Flow Calculations,*26th Symposium on Naval Hydrodynamics*, Rome, Italy, September 2006.

[18] Jovic, S., Driver, D. M., Backward-Facing Step Measurements at Low Reynolds Number, *NASA Technical Memorandum 108807*, Ames Research Center, February 1994.

[19] Spalart, P.R., Allmaras, S.R., A One-Equation Turbulence Model for Aerodynamic Flows, *AIAA 30$^{\text{th}}$ Aerospace Sciences Meeting*, Reno, January 1992.

[20] van der Ploeg, A., Eça, L., Hoekstra, M., Combining Accuracy and Efficiency with Robustness in Ship Stern Flow Computation, *23$^{\underline{\text{rd}}}$ Symposium on Naval Hydrodynamics*, Val de Reuil, France, September 2000.