

CFD Uncertainty Analysis for Turbulent Flows using Error Equation Method

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1 Introduction

In the recent past years, the CFD community has made a growing endeavour to quantify the uncertainty of numerical computations (known as Verification of calculations) as detailed and justified for example in [8,1,3]. Following this essential effort, the present workshop considers two test cases of 2-D, steady, incompressible, turbulent flows from the ERCOFTAC Classic Database (Case 18 and 30) to test error estimation procedures in practical applications. An interesting classification of these procedures can be found in [7]. Many of them, proposed in the literature, are based on grid refinement studies along with Richardson extrapolation. Successes, difficulties and failures of such a methodology have already been pointed out for example in [1,2]. This paper intends to present an alternative technique based on an equation for the discretization error in order to take into account its known transport properties and making this approach a single grid error estimator. This methodology has already been developed and applied with great success for laminar flows in [3]. We are interested here to extend it to the treatment of practical turbulent flows using the Spalart-Allmaras turbulence model [9].

2 Presentation of the flow solver

The ISIS flow solver, developed in our laboratory, uses the incompressible Reynolds-Averaged Navier-Stokes equations. The solver is based on the finite-volume method to build the spatial discretization of the transport equations on unstructured grids. The face-based method is generalized to unstructured meshes composed of arbitrary volume shapes. The velocity field is obtained from the momentum conservation equation and the pressure field is extracted from the mass conservation constraint transformed into a pressure equation. Picard's procedure is used for the linearization of the equations. The whole discretization is fully implicit in space and time and is formally second order accurate.

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Several near-wall low-Reynolds number turbulence models, ranging from one-equation Spalart-Allmaras model, two-equation $k - \omega$ closures, to a full Reynolds stress transport $R_{ij} - \omega$ model are implemented in the code. For all the computations considered here, the Spalart-Allmaras model [9] is used without transition terms.

Different methods are also available for solving linear systems. In this study, PGMRES method with ILU-k preconditioning is considered. More details on the numerical methods and their implementations can be found in [3].

3 The error equation method

3.1 Introduction

The present section is dedicated to the error estimation method used in this study. The error considered here is called discretization error. It involves the discretization of the equations which are to be solved as well as the discretization of the geometry and the boundary conditions which create an error due to incomplete grid convergence and imperfect grid generation (grid aspect ratio, skewness, non orthogonality). Letting ϕ be the exact solution which satisfies the differential operator \mathcal{N} representing the PDE governing this conserved variable, and a grid G_h of size h from which a numerical solution ϕ_h (p^{th} order accurate solution) is computed with the ISIS code, then the discretization error is defined as :

$$e_h = \phi - \phi_h \quad (1)$$

The method of the equation for the error is based on the construction of a problem for the discretization error e_h associated to the discrete solution ϕ_h . Solving this problem on the grid G_h leads to an estimation of the discretization error which is potentially influenced by the whole computational domain as the known transport properties of the error are taken into account. Thus, the estimation is composed of a local contribution and a global contribution. The problem for the error is derived using the continuous problem and the discretization error definition (1).

Similar methodologies have already been used in the literature with two different namings which are *Discrete Error Transport Equation* methods and *Defect Error Correction* methods as detailed in [3] (see e.g. [11,6,4,5]). Despite this semantic difference, these methods are completely equivalent although the first kind of methodology is designed for the purpose of error estimation and the second kind for the purpose of higher order estimation of solutions. This equivalence arises as having a r^{th} order accurate estimation of the error on a p^{th} order accurate solution ($r > p$) is equal to have a r^{th} order accurate solution (with no error estimation on it) by correcting the p^{th} order accurate solution with the r^{th} order accurate estimation of the error using the superconvergence property of the method.

The present implementation of the method of the equation for the error designed for finite-volume method on unstructured meshes has been extensively presented and studied in [3]. Its properties have been pointed out on analytical problems using the Method of the Manufactured Solution [8,3]. And it has been used successfully for estimating the errors on numerical solutions of laminar flows. For the sake of brevity, this section will only

present the main results and will focus more precisely on the treatment of the turbulence model.

3.2 Errors on the Navier-Stokes Equations

The adimensional form of the bidimensional incompressible Reynolds-Averaged Navier-Stokes equations, with a first order turbulence closure, can be summerized using differential operators \mathcal{N} and \mathcal{D} and classical notations :

$$\mathcal{N}(u, p, \nu_t) = \vec{\nabla} \cdot (\vec{U} u) - \vec{\nabla} \cdot \left[\left(\frac{1}{\text{Re}} + \nu_t \right) \vec{\nabla} u \right] + \vec{\nabla} p \cdot \vec{i}_x = 0 \quad (2a)$$

$$\mathcal{N}(v, p, \nu_t) = \vec{\nabla} \cdot (\vec{U} v) - \vec{\nabla} \cdot \left[\left(\frac{1}{\text{Re}} + \nu_t \right) \vec{\nabla} v \right] + \vec{\nabla} p \cdot \vec{i}_y = 0 \quad (2b)$$

$$\mathcal{D}(\vec{U}) = \vec{\nabla} \cdot (\vec{U}) = 0 \quad (2c)$$

For the moment, no particular turbulence model is considered for determining the unknown ν_t . Solving these equations and the ones related to the turbulence model with the ISIS code leads to a discrete solution for the velocity field $\vec{U}_h = (u_h, v_h)$, for the pressure p_h and for the turbulent kinematic viscosity $(\nu_t)_h$. According to the definition of the discretization error, the following decompositions can be written :

$$u = u_h + E_h^u \quad v = v_h + E_h^v \quad p = p_h + E_h^p \quad \nu_t = (\nu_t)_h + E_h^{\nu_t} \quad (3)$$

Errors on the components of the velocity field are components of the error on the velocity vector $\vec{E}_h = (E_h^u, E_h^v)$, so that $\vec{U} = \vec{U}_h + \vec{E}_h$. Using the previous decompositions in equations (2) leads to continuous equations for the errors that are linearized using Newton's procedure [3] :

$$\begin{aligned} & \vec{\nabla} \cdot (\vec{U}_h E_h^u) - \vec{\nabla} \cdot \left[\left(\frac{1}{\text{Re}} + \nu_t \right) \vec{\nabla} E_h^u \right] + \vec{\nabla} \cdot (\vec{E}_h u_h) \\ & - \vec{\nabla} \cdot (E_h^{\nu_t} \vec{\nabla} u_h) + \vec{\nabla} E_h^p \cdot \vec{i}_x = -\mathcal{N}(u_h, p_h, (\nu_t)_h) \end{aligned} \quad (4a)$$

$$\begin{aligned} & \vec{\nabla} \cdot (\vec{U}_h E_h^v) - \vec{\nabla} \cdot \left[\left(\frac{1}{\text{Re}} + \nu_t \right) \vec{\nabla} E_h^v \right] + \vec{\nabla} \cdot (\vec{E}_h v_h) \\ & - \vec{\nabla} \cdot (E_h^{\nu_t} \vec{\nabla} v_h) + \vec{\nabla} E_h^p \cdot \vec{i}_y = -\mathcal{N}(v_h, p_h, (\nu_t)_h) \end{aligned} \quad (4b)$$

$$\vec{\nabla} \cdot (\vec{E}_h) = -\mathcal{D}(\vec{U}_h) \quad (4c)$$

During the Newton's linearization only terms involving products of error have been neglected. It has been shown that this linearization approximation has no influence on the accuracy of the estimated error [3]. The main difference between the constructed problem for the error (4) and the primal one (2) is the presence of additional source terms which correspond to the *differential residuals* (the exact operator applied to the discrete solution). These extra source terms arise from *the truncation of functions* that appeared in \mathcal{N} and \mathcal{D} during the discretization step of (4). They are responsible for the local rise/decrease

of the error on the computational domain. Besides, it can be observed from equations (4) that discretization errors are driven by *similar transport rules* to solutions they referred to.

The differential residuals involve the continuous operators so that they can not be computed exactly. It is thus necessary to formulate an approximation of them which obviously should be more accurate than the discrete operators used in the flow solver (otherwise, it would correspond to the algebraic residuals which are reduced to zero machine during the computation). Using bicubic polynomials, a smooth r^{th} order accurate reconstruction ($r > p$), noted R_* , is applied to the discrete solutions. The differential residuals are then evaluated by the mean of the reconstructed solutions as all the derivatives present in the operators \mathcal{N} and \mathcal{D} can be computed. It should be noted that the reconstructed solutions have to be consistent with the boundary conditions of the original problem. And, in the case of finite-volume methods, the integration of the equations must be also r^{th} order accurate to keep the accuracy of the evaluated residuals. All the volume integrals over the control volumes involved can be transformed in surface integrals using the Green-Ostrogradsky's theorem and integration over faces is performed by the Simpson's rule. The higher order reconstruction and integration procedures developed have been described in details in [3] and they have been shown to be fourth order accurate ($r = 4$). As a result, the source terms in equations (4) are approximated by :

$$\mathcal{N}(u_h, p_h, (\nu_t)_h) \approx \mathcal{N}(R_*(u_h, p_h, (\nu_t)_h))$$

$$\mathcal{N}(v_h, p_h, (\nu_t)_h) \approx \mathcal{N}(R_*(v_h, p_h, (\nu_t)_h))$$

$$\mathcal{D}(\vec{U}_h) \approx \mathcal{D}(R_*(\vec{U}_h))$$

The equations for the errors (4) are solved numerically with a e^{th} order accurate method. Actually, their resolutions are performed using the same methods than the ones developed for the flow solver so that : $e = p = 2$. But, as explained in [5,3], the order of the approximate error is determined not by the order e of the discrete operator used to computed it, but by the order r of accuracy of the evaluated differential residual in (4). Generally speaking, the accuracy of the error estimation is given by the following relation : $p + \min(e, \min(p, r))$. Consequently, a fourth order accurate estimation of the discretization error is expected. Besides, the boundary conditions for the error are easy to derive. For a Neumann condition implemented on a variable, a free outlet boundary condition is applied to the corresponding error. And, for a Dirichlet condition, the error is naturally set to zero [3]. Finally, it should be emphasized that the estimation of the discretization errors are computed on *the same grid* than the numerical solutions themselves.

3.3 Extension to turbulent flow

The present section is devoted to present the extension of the error equation method for turbulent flows. Equations (4) involve the error $E_h^{\nu_i}$ on $(\nu_t)_h$. This term has to be computed using an equation for it, derived from the equations of the turbulence model used. In this

study, the one equation model of Spalart and Allmaras is considered without transition terms and with a near-wall low-Reynolds number formulation. Its defining adimensional equations are as follows :

$$\nu_t = f_{v1} \tilde{\nu} \quad (6a)$$

$$\begin{aligned} \mathcal{T}(\vec{U}, \tilde{\nu}) = & \vec{\nabla} \cdot (\vec{U} \tilde{\nu}) - \frac{1}{\sigma} \left[\vec{\nabla} \cdot \left[\left(\frac{1}{\text{Re}} + \tilde{\nu} \right) \vec{\nabla} \tilde{\nu} \right] \right] - c_{b1} \tilde{S} \tilde{\nu} \\ & - \frac{c_{b2}}{\sigma} \left[\vec{\nabla} \tilde{\nu} \cdot \vec{\nabla} \tilde{\nu} \right] + c_{w1} f_w \left(\frac{\tilde{\nu}}{d} \right)^2 = 0 \end{aligned} \quad (6b)$$

where d is the distance from the closest surface. The different constants and functions that appeared in (6) can be found in [9] or [10]. Once again the decompositions (3) are introduced in (6) in order to write an equation for $E_h^{\nu_t}$ which is linearized in the Newton's sense. When deriving this equation, the different functions (f_{v1} , f_w and \tilde{S}) of equations (6) are considered as part of the model and thus it is supposed that no errors are attached to their discretisations. This consideration leads to great simplifications in the equation for the error even though it is the only justification to it and it is not possible to evaluate the influence of such an approximation. Finally, the following equations hold :

$$E_h^{\nu_t} = f_{v1} E_h^{\tilde{\nu}} \quad (7a)$$

$$\begin{aligned} & \vec{\nabla} \cdot (\vec{U}_h E_h^{\tilde{\nu}}) - \frac{1}{\sigma} \left[\vec{\nabla} \cdot \left(\left(\frac{1}{\text{Re}} + \tilde{\nu}_h \right) \vec{\nabla} E_h^{\tilde{\nu}} \right) \right] + \vec{\nabla} \cdot (\vec{E}_h \tilde{\nu}_h) \\ & - \frac{1}{\sigma} \vec{\nabla} \cdot (E_h^{\tilde{\nu}} \vec{\nabla} \tilde{\nu}_h) - c_{b1} \tilde{S} E_h^{\tilde{\nu}} - \frac{c_{b2}}{\sigma} (\vec{\nabla} E_h^{\tilde{\nu}} \cdot \vec{\nabla} E_h^{\tilde{\nu}}) \\ & - 2 \frac{c_{b2}}{\sigma} (\vec{\nabla} E_h^{\tilde{\nu}} \cdot \vec{\nabla} \tilde{\nu}_h) + \frac{2 c_{w1} f_w \tilde{\nu}_h}{d^2} E_h^{\tilde{\nu}} = -\mathcal{T}(\vec{U}_h, \tilde{\nu}_h) \end{aligned} \quad (7b)$$

As before the differential residual $\mathcal{T}(\vec{U}_h, \tilde{\nu}_h)$ is evaluated using fourth order approximation. A fourth order reconstruction operator is applied to the numerical solutions and fourth order accurate integrations are performed as required by the finite-volume method. Concerning this last step and unlike previously, all the volume integrals that are part of $\mathcal{T}(\vec{U}_h, \tilde{\nu}_h)$ can not be transformed in surface integrals. The integration over control volumes is performed using a local transformation to a generalized coordinate space which corresponds to a local analytic bilinear description of the volumes. Functions to be integrated are considered as bicubic polynomials expressed in generalized coordinates. This procedure ensures fourth order integration over control volumes.

In order to compute $E_h^{\nu_t}$, equation (7b) is solved, with the same method than for (6b) in the ISIS solver, along with the previous error equations.

3.4 Conclusion

The method of error estimation introduced in this section presents a number of interesting features that are detailed in [3]. First and foremost, the error estimator is monogrid so that the error can be evaluated along with the variable solved. Furthermore, no hypothesis is imposed neither on the accuracy of the considered solutions nor on the size of the grids used even though the method is more effective on fine meshes since the differential residuals

involve only the first truncated terms on such grids. Besides, it should be pointed out that this method does not require any normalization step as it is the case for some other error estimators [3].

However, the main disadvantage of this methodology comes from the relative complexity of its implementation which requires the use of higher order numerical methods for computing the differential residuals. Hopefully, error equations can be solved using similar numerical techniques than for the flow solver. It should be also emphasized that the equations for the errors solved are linear (but coupled) leading theoretically to CPU time requirement really lower than for solving the primal problem.

This method has yielded fourth order accurate error estimations ($p = e = 2$ and $r = 4$) for laminar flows in [3]. Furthermore, this methodology brings not only estimation of errors but also estimation of source terms of errors which indicates where and how error is produced over the computational domain. Using these informations for guiding a h-adaptive method has shown to be even more efficient (in term of error reduction) than using the exact error itself.

4 Results

This workshop considered two different test cases from the ERCOFTAC Classic Database : the 2D model Hill flows (Case 18) and the 2D Backward-Facing Step (Case 30). The results of numerical evaluations of local and integral quantities of interest and their error estimations are provided on a separated document. This section is dedicated to present the characteristic results of the previously presented error estimation method. For the sake of brevity, only the 2D Backward-Facing Step test case will be considered here for illustrating the main features of the methodology.

The first section will give some details concerning the performed computations with the ISIS code for this workshop. The second section intends to use the so-called Richardson extrapolation method as it is undoubtedly the most widespread methodology for error estimation in the CFD community. And the last section is relative to the results of the error equation method.

4.1 Presentation of the computations

All the computations were performed with the ISIS flow solver presented in section 2. A no-slip boundary condition is prescribed at the walls of all the computational domains. At the outlet, a Neumann boundary condition is applied on the velocity components and on $\tilde{\nu}$ ensuring a zero gradient flux through these boundaries. And a Dirichlet condition sets the pressure to zero. At the inlet, Dirichlet boundary conditions are applied to all quantities by the mean of the inlet profiles provided for this workshop, except for the pressure on which a zero gradient flux is imposed. For each set of grids the discrete profile on the finest mesh locally fourth order reconstructed is considered as the exact profile so that the *exact* value of variables can be computed anywhere at the inlet boundary (this is required for the evaluation of the differential residuals).

For all the computations, the algebraic residual of each equation solved is reduced to zero machine in double precision. Thus, iterative errors are negligible compared to discretization errors.

During the post-processing of the data, any interpolation needed is done using fourth order accurate reconstruction instead of second order one in order not to pollute solutions with noise of the same order than their accuracies (that are expected to be around order 2 using the ISIS code). And, for computing integral quantities, second order accurate integrations are performed.

4.2 Richardson extrapolation method

This section is devoted to a short analysis of the Richardson extrapolation method for error estimation. Concerning the Verification of a particular computation, this methodology is clearly the most widespread in the open literature. It has been presented, applied and analysed on different test cases in [3] along with a detailed bibliography.

From this study, it has been shown that this method gives very good results for simple academic numerical test cases leading to third order accurate error estimation (for second order accurate solution) in the asymptotic range. However, this method is much more limited regarding more complex applications since it strictly required a monotonic convergence (and solutions on at least three different grids in the asymptotic range with no iteration errors on them (!)) that can not always be ensured making the extrapolation impossible. Once again this feature appeared in the present task of error estimation for some quantities of interest so that no error estimation can be computed.

Furthermore, even if the right behaviour of the convergence of a quantity is observed, the error estimation can still be troublesome as pointed out in [1]. The difficulty arises from the dispersion of values used for the extrapolation. As an example, the re-attachement point values for the backward-facing step computed on the grids of set B is considered (see table 1). It is intended here to estimate the discretization error on the re-attachement point value computed on the finest grid (Grid 7). As it can be observed in table 2, the error estimation (and the apparent order of convergence) is dependent on the set of grids selected for the extrapolation even if only the finest ones are considered.

Grid	$Nx * Ny$	h_i/h_1	NCell	X(Rea)
1	101x101	2.40	10000	6.58962
2	121x121	2.00	14400	6.49893
3	141x141	1.71	19600	6.41447
4	161x161	1.50	25600	6.34579
5	181x181	1.33	32400	6.28802
6	201x201	1.20	40000	6.24037
7	241x241	1.00	57600	6.17379

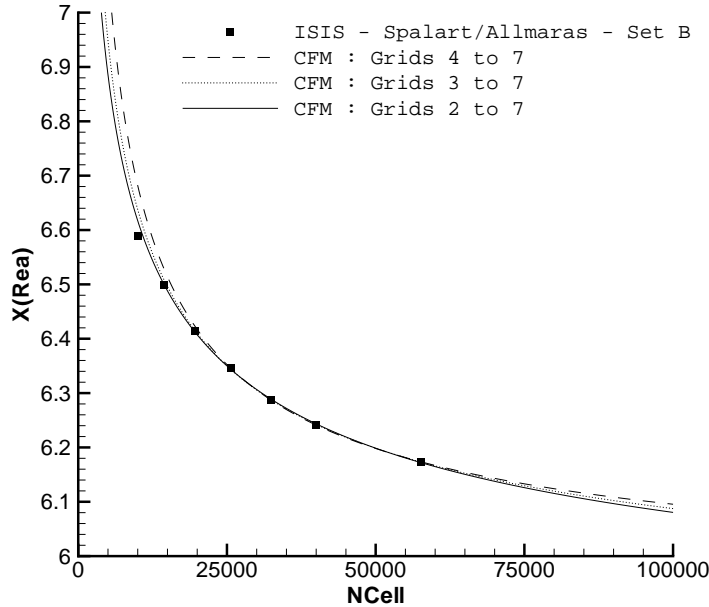
Table 1. Results (Set B) : Re-attachement point

Grids	p	Err ^a
5-6-7	1.50	0.21172
4-6-7	1.26	0.25689
4-5-7	1.06	0.32108
3-5-7	0.88	0.39591
1-4-7	0.46	0.84145

Table 2. Richardson extrapolation for the re-attachement point

^a on the solution from Grid 7

In order to overcome this difficulty, Eça *et al.* have proposed a least square approach of the Richardson extrapolation method known as the *Curve Fit Method* (CFM) that is presented and explained in [1]. This methodology permits the treatment of data with highly scattered results. But the CFM is still dependant on the sets of grids used for computing the fitted curves as it can be observed in table 3 (see also figure 1).



Grids	p	Err ^a
4 to 7	1.18	0.28206
3 to 7	0.89	0.39259
2 to 7	0.71	0.51524

Table 3. Curve Fit Method for the re-attachment point

Fig. 1. Data and fitted curves relative to table 3

^a on the solution from Grid 7

It should be noted that these trends regarding this methodology can even be more impressive for other quantities or other set of grids. Difference of more than two orders of magnitude have been observed in the estimated errors on a solution. These results emphasized the need for applying safety factors on the estimated error from Richardson extrapolation as proposed by Roache [8]. However, such a practice is not completely satisfactory in term of precise discretization error estimation.

4.3 Error Equation method

This section presents the results of the error equation method applied to the 2D Backward-Facing Step (Case 30). Computations have been performed on the seven grids of Set A which ranged from 10000 cells to 57600 cells (as for Set B, see table 1). Thus, the finest mesh is not *very fine* for a 2D turbulent flow. Besides, the quality of the grids of this set is relatively poor near the step as it can be seen on figure 2 making this test case quite difficult in term of error estimation. Generally speaking, the quality of the results of error estimation is difficult to evaluate since no exact solution (and thus no exact error) is available. We first consider the error norms (L_1) of the different variables on figure 4 along with the corresponding norms of the differential residuals (which are the source terms of error) on figure 3. It can be seen that the convergence of error norms is similar for all the quantities. Table 4 gives the apparent orders of convergence of the variables as computed

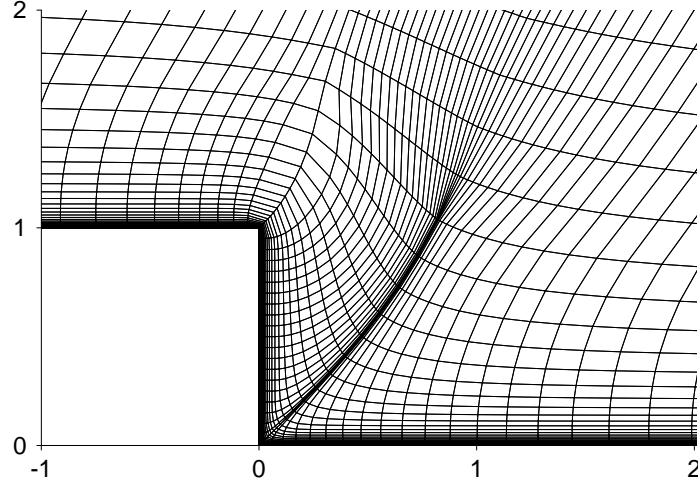


Fig. 2. Mesh in the vicinity of the step (Grid 1)

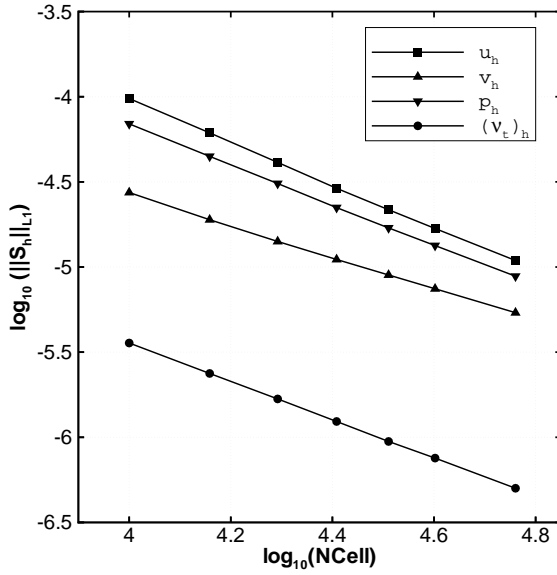


Fig. 3. Convergence of Differential Residuals

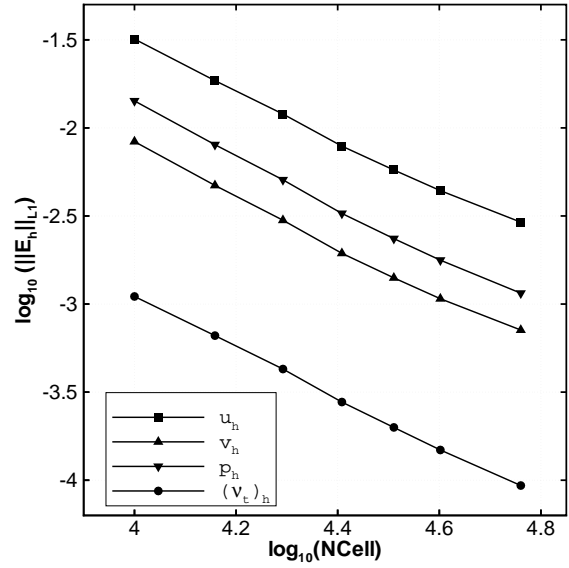


Fig. 4. Convergence of Errors

from the slopes of curves from figure 4. It can be observed that the apparent orders seem to converge to values near from theoretical orders that are located around 2. This result is thus consistent with what was expected even though it is definitely not a proof of the efficiency of the present methodology. The slopes for differential residuals have a similar behaviour as expected from theory (the theoretical slope is $\min(p, r-n)$ where n is the order of the considered operator that is always 2 in this study). However, this analysis indicates that the so-called asymptotic range is not reached for the grids considered in this study.

Grids	$p[u_h]$	$p[v_h]$	$p[p_h]$	$p[(\nu_t)_h]$
1-2	2.981	3.142	3.141	2.806
2-3	2.835	2.954	2.982	2.834
3-4	3.139	3.237	3.291	3.232
4-5	2.648	2.725	2.792	2.815
5-6	2.558	2.589	2.676	2.798
6-7	2.262	2.244	2.369	2.550

Table 4. Convergence of apparent orders of convergence

Figures 5 give the error fields computed on the finest grid of the considered set (\log_{10} of absolute values of errors). As expected, the maximum error is located in the vicinity of the step. As confirmed from the fields of the source terms, the upper corner of the step is responsible for the maximum of error production. From there, errors are convected and diffused inside the computational domain.

We now consider some local and integral flow quantities on figures 6 where the convergences of solutions are plotted along with the ones for extrapolated solutions (numerical solutions corrected with the evaluated errors). The area between these two curves is the error zone for each of the variables considered. For the coarsest grid, the error estimation may be poor.

Finally, it should be emphasized that the error estimation has a cost in term of CPU time requirement. Even though all the equations considered in this methodology are linear, they are coupled so that some coupling iterations have to be performed using the solving methodology linked to numerical methods of the ISIS flow solver. Considering that the cost of a non-linear/coupling iteration for the primal problem is similar to the one of a coupling iteration for the error problem, the error estimation costs between 6 and 7 time less than the computation of flow variables.

5 Conclusion

The error equation method has been presented in this paper for turbulent flows. The main difference from the treatment of laminar flows as detailed in [3] is obviously the estimation of error for the turbulent viscosity. When deriving an equation for it, the same methodology was applied than for the Navier-Stokes equations. Actually, an additional assumption has been made considering that the coefficients of the equation for $\tilde{\nu}$ are exact. This approximation has to be evaluated in order to determine its influence in the whole error problem. However, as pointed out previously, the results of an error estimator are difficult to quantify without an exact error solution available. Therefore, it is clear that only the Method of the Manufactured Solution would provide a suitable framework for such an evaluation. Nevertheless, the first results presented here are encouraging since they correspond to what can be expected.

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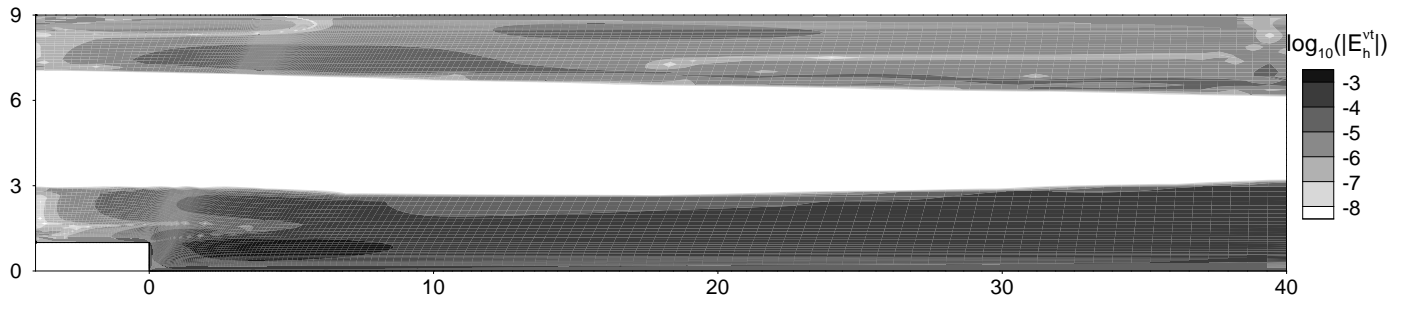
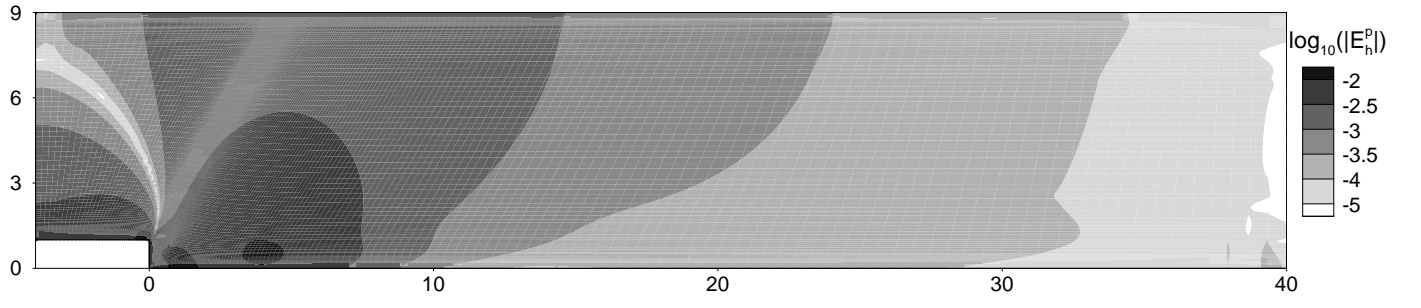
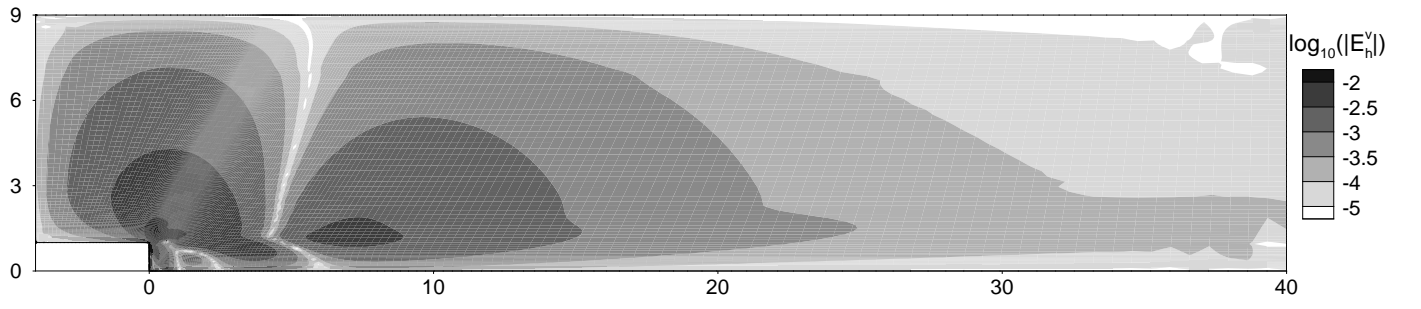
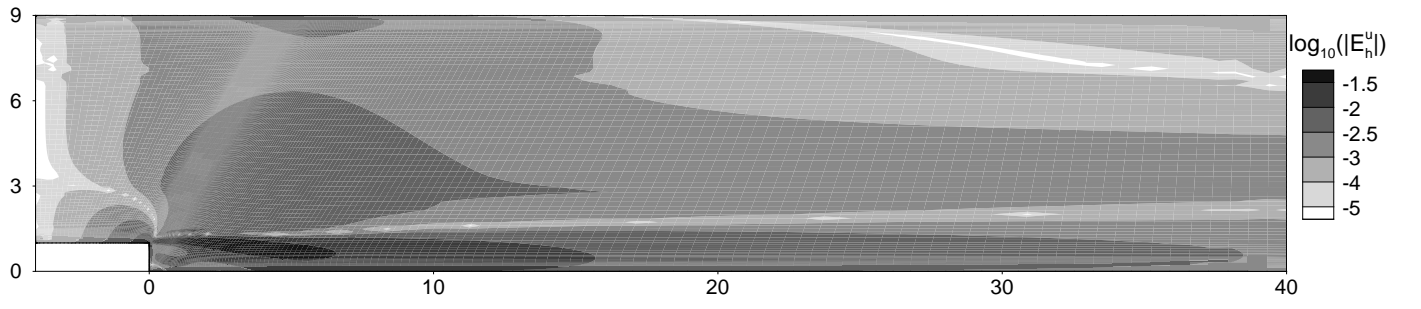
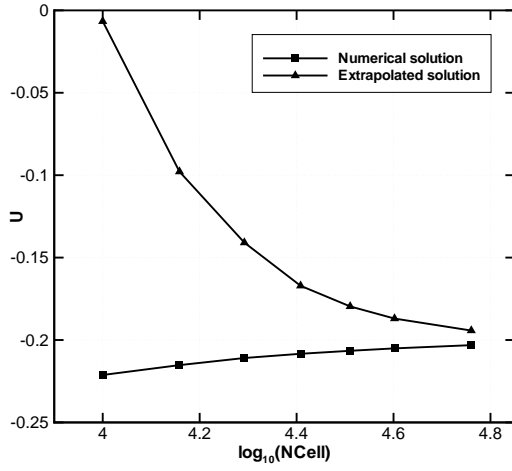
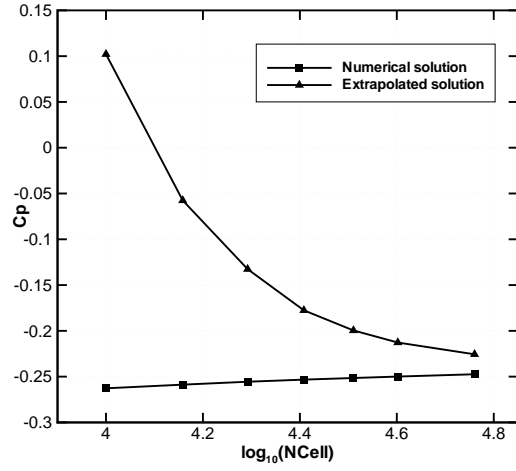


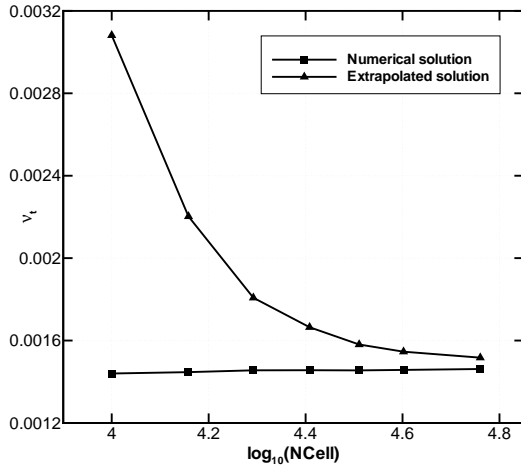
Fig. 5. Error fields on Grid 7 (241x241)



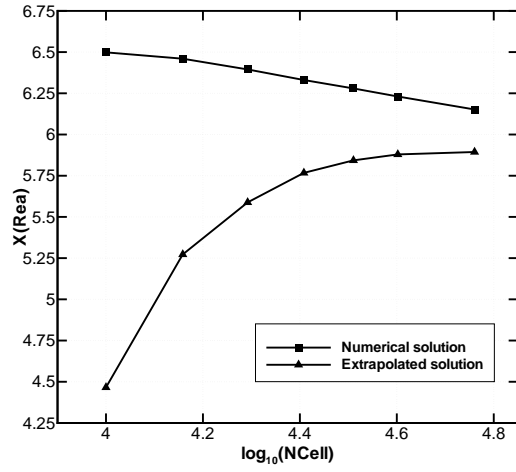
(a) U at $(X, Y) = (1, 0.1)$



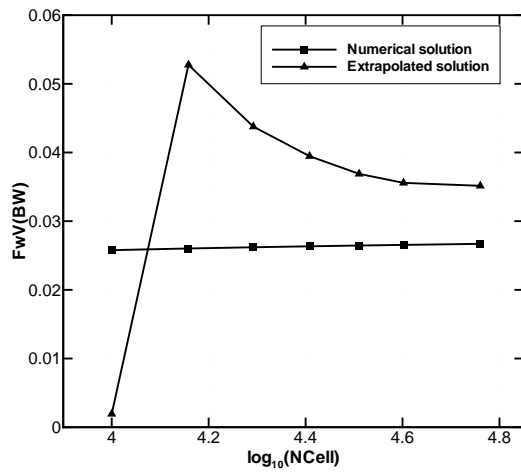
(b) C_p at $(X, Y) = (1, 0.1)$



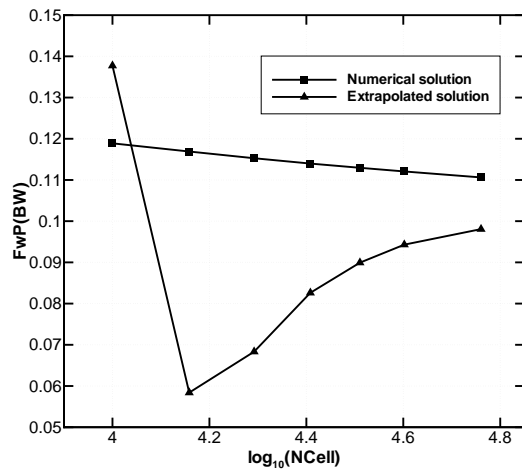
(c) ν_t at $(X, Y) = (1, 0.1)$



(d) Re-attachement point



(e) Friction resistance on bottom wall



(f) Pressure resistance on bottom wall

Fig. 6. Comparison of convergence of numerical and extrapolated solutions