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AN INTRODUCTION TO CFD CODE VERIFICATION INCLUDING EDDY-VISCOSITY MODELS

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Abstract. *This paper addresses the method of manufactured solutions for RANS solvers, i.e. in the context of the calculation of incompressible turbulent flows with eddy-viscosity turbulence models. The difficulties caused by damping and/or blending functions included in the turbulence models are discussed. The need to manufacture the turbulence quantities included in the turbulence models is illustrated with an example for the Spalart & Allmaras one-equation model.*

1 INTRODUCTION

The maturing of CFD codes for practical calculations of complex turbulent flows implies the need to establish the credibility of the results by Verification & Validation. Because the discussion about these important subjects is ongoing in several forums, like for example the AIAA[1], the ERCOFTAC[2] or the ITTC Resistance Committee[3], it is possible to find different definitions of Verification and Validation. However, a clear and simple definition is given by Roache[4]: Verification is a purely mathematical exercise that intends to show that we are "solving the equations right", whereas Validation is a science/engineering activity that intends to show that we are "solving the right equations".

Verification is in fact composed of two different activities[4]: Code Verification and Verification of Calculations. Code Verification intends to verify that a given code solves correctly the equations of the model that it contains by error evaluation. On the other hand, Verification of Calculations intends to estimate the error of a given calculation, for which in general the exact solution is not known. Verification of Calculations should be preceded by Code Verification and this was one of the main conclusions of the first workshop on uncertainty analysis, held in Lisbon in 2004[5,6].

The evaluation of errors required by Code Verification implies that the exact solution must be available. In complex turbulent flows, this condition cannot be met. The only option left then to perform Code Verification is applying the Method of the Manufactured Solutions (MMS)[4,7,8,9,10,11,12]. In the MMS, a continuum solution is first constructed, i.e. one specifies all unknowns by mathematical functions. In general, this constructed solution will not satisfy the governing equations (continuity and momentum) because of the arbitrary nature of the choice. But by adding an appropriate source term, which removes any imbalance caused by the choice of the continuum solution, the governing equations are forced to become a model for the constructed solution.

In the MMS, the constructed solution need not have a physical meaning, since Verification (of codes or of calculations) is a purely mathematical exercise. However, as suggested by Eça *et al.*[13], choosing a physically realistic manufactured problem which has a closed form solution offers several advantages. First, it exercises each term involved in the PDE in a manner similar to that of a real problem so that similar difficulties in the solution and error estimation processes will arise. Secondly, using a physically realistic manufactured solution leads to smaller source terms so that the PDE does not tend towards a degenerate form controlled by the magnitude of the source terms. Finally, it makes the methodology more attractive for the engineering community.

Once a suitable MS is available, the actual verification process can start. One solves the governing equations with added source terms on a domain in which the MS is valid, using boundary conditions which are valid in the MS. Typically one intends then to demonstrate that the error with respect to the constructed solution tends to zero with grid refinement and that the observed order of accuracy corresponds to the theoretical order of the discretisation technique used. If unexpected behaviour occurs, further investigations are needed to detect the source of the problem. This might even involve freezing individual terms of the equations by replacing them with the exact solution. Thus the term responsible for the trouble may be identified.

A proper code verification should make sure that all terms in the equations are exercised, which puts demands on the MS itself but also requires for instance that solutions are obtained on non-orthogonal grids.

The present paper presents in section 2 a discussion about the construction of manufactured solutions for testing RANS solvers, i.e. CFD codes operating with eddy-viscosity turbulence models. Section 3 discusses the problem of error evaluation in grid refinement studies and section 4 presents one example of Code Verification including the Spalart & Allmaras[14] one-equation turbulence model. The final remarks of the paper are presented in section 5.

2 MANUFACTURED SOLUTIONS FOR RANS SOLVERS

In the calculation of the incompressible turbulent flows with eddy-viscosity turbulence models, the solution of the continuity and momentum equations do not form a closed system of equations. Where algebraic turbulence models are hardly used these days,

transport equations for one or two turbulence quantities have to be solved in order to determine the eddy-viscosity. Therefore, a manufactured solution (MS) for a RANS solver should include also manufactured turbulence quantities.

This seems a straightforward exercise because the philosophy of the MMS is the same: one defines the turbulence quantities with a mathematical function and a source term is added to the transport equation(s) to cancel any imbalance originated by the chosen function(s). However, there are problems in this specification due to the existence of damping and/or blending functions in many of the most popular turbulence models and due to the highly non-linear character of the transport equations for the turbulence quantities. As discussed by Knupp and Salari[11], this latter aspect may even raise the problem of non-uniqueness of the solution.

As an illustration of the problems that one may encounter to construct manufactured solutions for Code Verification of eddy-viscosity turbulence models, we have selected the MS proposed by Eça *et al.*[13], which defines the eddy-viscosity as

$$\nu_t = 0.25 \nu_{max} \eta_\nu^4 e^{2-\eta_\nu^2} \tag{1}$$

in a squared domain with $0.5 \leq x \leq 1$ and $0 \leq y \leq 0.5$.

$$\eta_\nu = \frac{\sigma_\nu y}{x}, \quad , \sigma_\nu = 10 \ \text{ and } \ \nu_{max} = 10^3 \nu.$$

$\nu = 10^{-6} U_1 L$, where L and U_1 are the length and velocity reference scales.

2.1 One-equation eddy-viscosity models

In the one-equation models of Spalart & Allmaras[14] and Menter[15], the eddy-viscosity is defined by the product of the dependent variable of the model and a damping function. In the Spalart & Allmaras model[14] ν_t is given by

$$\nu_t = \tilde{\nu} f_{v1} \tag{2}$$

with

$$f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3} \tag{3}$$

and

$$\begin{aligned} \chi &= \frac{\tilde{\nu}}{\nu} , \\ c_{v1} &= 7.1 . \end{aligned} \tag{4}$$

For the Menter[15] model, the eddy-viscosity is obtained from

$$\nu_t = D_2 \tilde{\nu}_t , \tag{5}$$

where

$$D_2 = 1 - e^{-\left(\frac{\tilde{\nu}_t}{A^+ \kappa \nu}\right)^2} \tag{6}$$

and

$$\begin{aligned} A^+ &= 13\,, \\ \kappa &= 0.41\,. \end{aligned} \tag{7}$$

If one specifies the eddy-viscosity and determines $\tilde{\nu}$ and $\tilde{\nu}_t$ from the definition equations (2) and (5), the first and second derivatives of $\tilde{\nu}$ and $\tilde{\nu}_t$ with respect to x and y will have to be determined implicitly. For example, for the dependent variable of the Spalart & Allmaras model, $\tilde{\nu}$, we have:

$$\begin{aligned} \frac{\partial \tilde{\nu}}{\partial x} &= \frac{\partial \nu_t}{\partial x}\frac{d\tilde{\nu}}{d\nu_t} \\ \frac{\partial \tilde{\nu}}{\partial y} &= \frac{\partial \nu_t}{\partial y}\frac{d\tilde{\nu}}{d\nu_t} \\ \frac{\partial^2 \tilde{\nu}}{\partial x^2} &= \frac{d\tilde{\nu}}{d\nu_t}\left[\frac{\partial^2 \nu_t}{\partial x^2} - \left(\frac{\partial \nu_t}{\partial x}\right)^2 \left(\frac{d\tilde{\nu}}{d\nu_t}\right)^2 \frac{d^2\nu_t}{d\tilde{\nu}^2}\right] \\ \frac{\partial^2 \tilde{\nu}}{\partial y^2} &= \frac{d\tilde{\nu}}{d\nu_t}\left[\frac{\partial^2 \nu_t}{\partial y^2} - \left(\frac{\partial \nu_t}{\partial y}\right)^2 \left(\frac{d\tilde{\nu}}{d\nu_t}\right)^2 \frac{d^2\nu_t}{d\tilde{\nu}^2}\right] \\ \frac{d\tilde{\nu}}{d\nu_t} &= \frac{1}{\frac{d\nu_t}{d\tilde{\nu}}} \end{aligned} \tag{8}$$

It is obvious that similar equations are obtained for $\tilde{\nu}_t$.

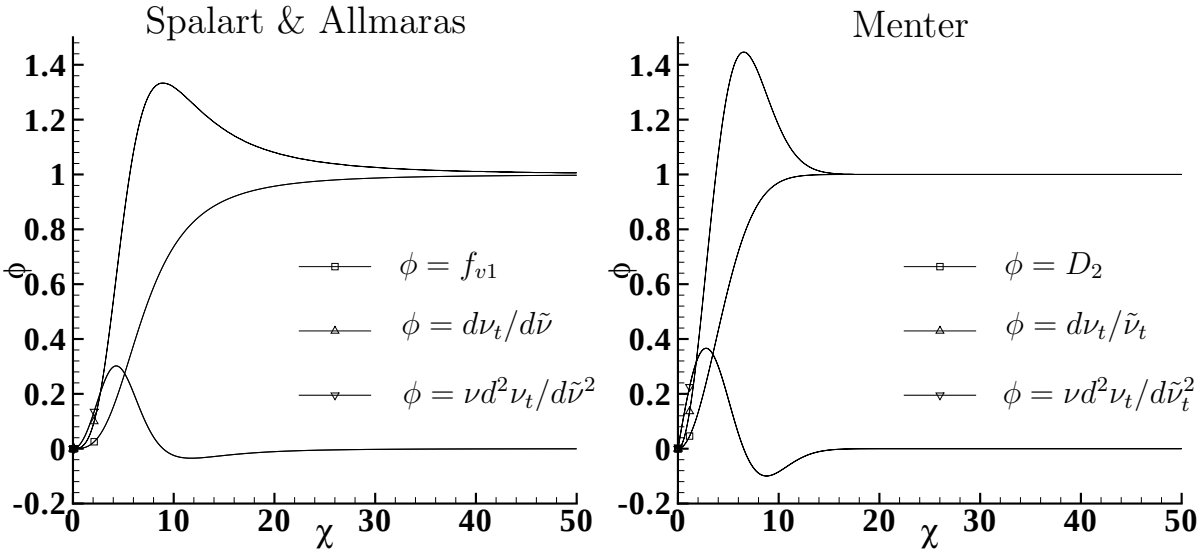

Figure 1: Damping functions and first and second derivatives of ν_t with respect to $\tilde{\nu}$ and $\tilde{\nu}_t$ for the one-equation turbulence models of Spalart & Allmaras and Menter.

The damping functions, f_{v1} and D_2, and the first and second derivatives of ν_t with respect to $\tilde{\nu}$ and $\tilde{\nu}_t$ are illustrated in figure 1. The second derivatives of ν_t have been

multiplied by ν to fit in the plots of figure 1. The second derivatives of ν_t with respect to $\tilde{\nu}$ and $\tilde{\nu}_t$ exhibit a very high peak value close to $\tilde{\nu} = \tilde{\nu}_t \simeq 4\nu$ (the plotted value has to be divided by ν). Therefore, the second derivatives of $\tilde{\nu}$ and $\tilde{\nu}_t$ included in the diffusion terms of the turbulence quantities transport equations will be very difficult to capture numerically.

On the other hand, if one specifies $\tilde{\nu}$ and $\tilde{\nu}_t$ from equation (1), the first and second derivatives of $\tilde{\nu}$ and $\tilde{\nu}_t$ with respect to x and y will be perfectly smooth. The momentum equations include only the first derivatives of ν_t with respect to x and y. Therefore, the manufactured solution for the eddy-viscosity will still be smooth because the first-derivative of ν with respect to $\tilde{\nu}$ and $\tilde{\nu}_t$ does not exhibit any special difficulties. We conclude that a MS for RANS with a one-equation turbulence model is best set up with $\tilde{\nu}$ (or $\tilde{\nu}_t$) specified, rather than ν_t.

2.2 Two-equation eddy-viscosity models

For two-equation models the strategy proposed by Eça *et al.*[13] is to define the turbulence kinetic energy, k, the square root of which is the turbulence velocity scale of most of the two-equation eddy-viscosity turbulence models. The second dependent variable of the turbulence model, providing the turbulence length scale, follows from the definition of ν_t as a function of k and the second dependent variable. For instance in the $k-\epsilon$ model the second variable ϵ would be derived from

$$\epsilon = c_\mu \frac{k^2}{\nu_t}.$$

An elegant way to specify k is to use Bradshaw's hypothesis for turbulence in equilibrium, which defines k as a function of ν_t and the strain rate. However, this type of approach is more suitable for unconfined flows, because the turbulence quantities behaviour observed in near-wall turbulent flows cannot possibly be reproduced with it. To obtain a variation of k representative for what happens in near-wall turbulent flow Eça *et al.*[13] specified k as

$$k = k_{max} \eta_\nu^2 e^{1-\eta_\nu^2} \ , \tag{9}$$

where the proposed value of k_{max} is 0.01.

With the specification of ν_t and k from equations (1) and (9) it would seem easy to obtain the prescribed field of the second dependent variable for any of the two-equation turbulence models available in the literature. However, there are exceptions. Furthermore, there is no guarantee that the prescribed turbulence quantities will produce the expected behaviour of damping and/or blending functions included in the turbulence model.

In order to illustrate these two types of problems we have selected two popular versions of the two-equation $k-\omega$ model proposed by Menter[16]: the baseline (BSL) and the shear stress transport (SST) versions of the $k-\omega$ model.

In the SST $k-\omega$ model[16], ν_t is given by

$$\nu_t = \frac{a_1 k}{\max\left(a_1\omega, S_\Omega F_2\right)} \tag{10}$$

where

$$F_2 = \tanh\left(arg_2^2\right) \tag{11}$$

with

$$arg_2 = \max\left(2\frac{\sqrt{k}}{0.09\omega y}, \frac{500\nu}{\omega y^2}\right) \tag{12}$$

S_Ω is the magnitude of vorticity, y is the distance to the wall and $a_1 = 0.31$.

Alternatively, equation (10) may be written as

$$\nu_t = f_\omega \frac{k}{\omega} \tag{13}$$

where f_ω plays the role of a damping function given by

$$f_\omega = \min\left(1, \frac{a_1\omega}{S_\Omega F_2}\right) \ . \tag{14}$$

In the definition of ν_t, equation (10), ω is replaced by the vorticity magnitude in the regions where the eddy-viscosity definition guarantees that the shear-stress in a boundary-layer does not exceed $0.31k$. Therefore, in these regions ν_t becomes independent of ω and so one can not determine ω from ν_t and k, unless the limiter is never active and so the SST model reduces to the BSL version.

For the SST $k-\omega$ model it is possible to specify k and ω to obtain a MS. A simple example is constructed by specifying k as in equation (9) and ω by

$$\omega = \frac{k}{\nu_t} = 4\frac{k_{max}}{\nu_{max}} e^{-1} \eta_\nu^{-2} \ , \tag{15}$$

using equations (1) and (9). Figure 2 presents the profiles of ν_t and the function f_ω at seven x positions obtained from the k and ω defined by equations (9) and (15). The function f_ω makes it easy to identify the region where the eddy-viscosity limiter is active.

As illustrated in figure 2, the first derivatives of the eddy-viscosity are discontinuous at the locations where the limiter is turned on and off. In the context of a MS, this will be troublesome because the derivatives of ν_t, required for the calculation of the source terms of the momentum equations, are not uniquely defined at these locations.

In the BSL and SST versions of the $k-\omega$ model proposed by Menter[16], there is a blending function, F_1, which is given by

$$F_1 = \tanh\left(arg_1^4\right) \tag{16}$$

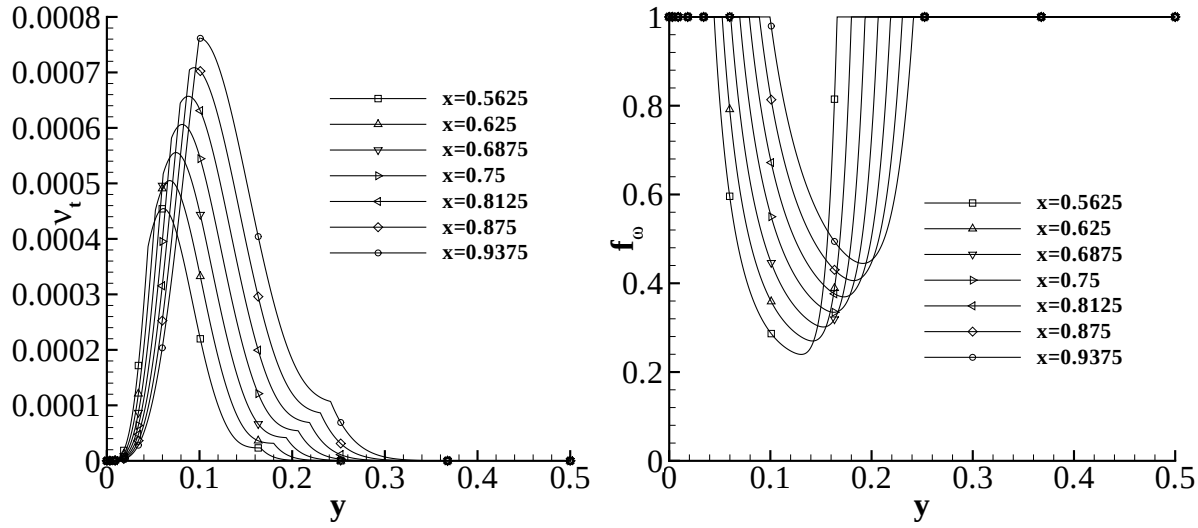

Figure 2: Eddy-viscosity and f_ω profiles at 7 x coordinates of a manufactured solution for the SST $k-\omega$ constructed from the k and ω fields.

where

$$arg_1 = \min\left[\max\left(\frac{\sqrt{k}}{0.09\omega y}, \frac{500\nu}{\omega y^2}\right), \frac{4k}{\sigma_{\omega 2} CD_{k\omega} y^2}\right] \tag{17}$$

and

$$CD_{k\omega} = \max\left(\frac{2}{\sigma_{\omega 2}\omega}\nabla k \cdot \nabla\omega, 10^{-20}\right) . \tag{18}$$

$\sigma_{\omega 2} = 1/0.856$.

The expected behaviour of F_1 in a "boundary-layer" is to be 1 in the "near-wall" region and to decay rapidly to 0 in the outer region. As illustrated in figure 3, there are several troublesome features in the F_1 profiles generated with the ν_t and k of equations (1) and (9):

- The F_1 profiles exhibit kinks and so the derivatives of F_1 with respect to x and y are not defined at these locations.
- The expected behaviour of a near-wall turbulent flow is not reproduced. F_1 is zero close to the bottom and it does not reach 1 for most of the computational domain.

The latter aspect is not a significant default, because one can still perform valid code verification without having the exact mimic of the F_1 behaviour. However, the first problem is troublesome because the derivative of F_1 is required for the calculation of the source term of the k and ω transport equations. Therefore, the problem is equivalent to the one discussed above for the eddy-viscosity definition in the SST model. As suggested by Eça *et al.*[13], for code verification purposes, one can avoid this problem by dropping the dependence of the coefficients of the diffusion terms of the k and ω transport equations

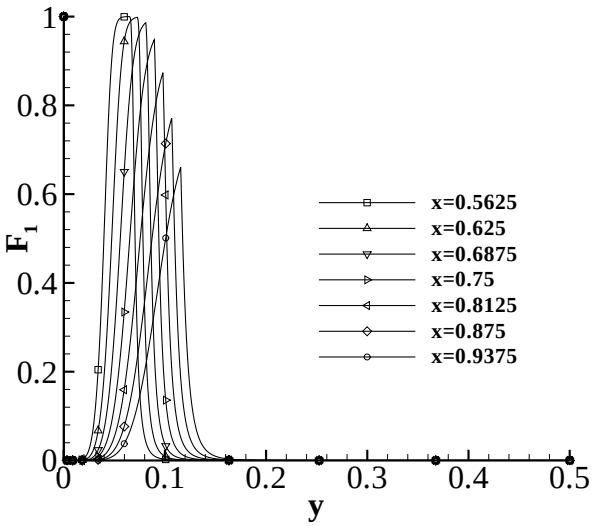

Figure 3: Profiles of the blending function, F_1, of the BSL and SST $k-\omega$ two-equation models at 7 x coordinates.

(σ_k and σ_ω) on the blending function, F_1. The awkward consequence is that one has to make a (small) change in the implementation of the turbulence model.

3 ERROR EVALUATION

It is commonly accepted[4] that the numerical error of a CFD prediction has three components: the round-off error, the iterative error and the discretization error. The round-off error is a consequence of the finite precision of the computers and its importance tends to increase with the grid refinement. The iterative error is originated by the non-linearity of the mathematical equations solved by CFD. In principle, one should be able to reduce the iterative error to the level of the round-off error. However, this may not always be possible with the increase of the grid density. The discretization error is a consequence of the approximations made (finite-differences, finite-volume, finite-elements,...) to transform the partial differential equations of the continuum approach into a system of algebraic equations. Unlike the other two error sources, the relative importance of the discretization error decreases with the grid refinement.

In code verification, one intends to demonstrate that the error of the solution tends to zero with the grid refinement and that the observed order of accuracy corresponds to the theoretical order of the discretization technique adopted. Therefore, it is important that the round-off and iterative errors are negligible compared to the discretization error.

The reduction of the round-off error is related to the number of digits available and to the numerical procedure performed to obtain the solution. In ill-conditioned problems, one may have difficulties to reduce the contribution of the round-off error, which is often the case for complex analytical solutions defined by infinite series expansions. However,

for smooth solutions the use of double-precision is usually sufficient to avoid any contamination of the round-off error. Obviously, there is a limit to the grid refinement imposed by the round-off error.

On the other hand, the reduction of the iterative error to negligible levels may be troublesome. There is no guarantee that a manufactured solution will converge easier than a practical complex turbulent flow. Therefore, it may be difficult to reduce the iterative error to a negligible level. It is likely that these difficulties depend on the selected MS and on the grid density. In such cases, the finest grid density may be determined by the behaviour of the iterative error.

The usual[4] representation of the discretization error of any flow quantity, ϕ, is a power series expansion where all high-order terms are neglected.

$$e(\phi) = \phi - \phi_{ms} \simeq \alpha h_i^p \ , \tag{19}$$

where the subscript $_{ms}$ identifies the manufactured solution, α is a constant, h_i is the typical cell size and p is the order of accuracy. The application of equation (19) requires the definition of a typical cell size, which is not always straightforward to do. A simple way to avoid ambiguities in the definition of h_i is the use of geometrically similar grids. However, in multi-block structured grids and unstructured grids this may not be easy to do.

It should be emphasized that there is no guarantee that the convergence of all the flow properties is uniform in the computational domain (i.e. p constant for all the field). Therefore, one should analyze the convergence of global (like the root mean square of the error) and local flow quantities. Furthermore, equation (19) assumes that the data are in the so-called 'asymptotic range' and experience tells that one should not trust the value of p obtained from the minimum number of grids required by equation (19) for its determination, which in this case is 2.

4 AN EXAMPLE OF CODE VERIFICATION FOR THE SPALART & ALLMARAS ONE-EQUATION MODEL

As an example of the importance of including the turbulence quantities transport equation on the code verification procedure, we have selected the MS proposed by Eça *et al.*[13] for the one-equation Spalart & Allmaras turbulence model. The MS is defined in a squared domain with $0.5 \leq x \leq 1$ and $0 \leq y \leq 0.5$, where x and y are the horizontal and vertical non-dimensional Cartesian coordinates.

The calculations were performed with the second-order accurate, 2-D, finite-differences version of PARNASSOS[17] in a set of 16 geometrically similar Cartesian grids with equidistant grid nodes in the x direction and clustered grid nodes close to the bottom boundary using a one-sided stretching function[18] (stretching parameter 0.05).

Figure 4 presents the root mean square (RMS) of the error of the horizontal velocity component u_x and ν_t as a function of the grid refinement ratio for three types of exercises: calculation of the eddy-viscosity field with the manufactured velocity field, U_{ms};

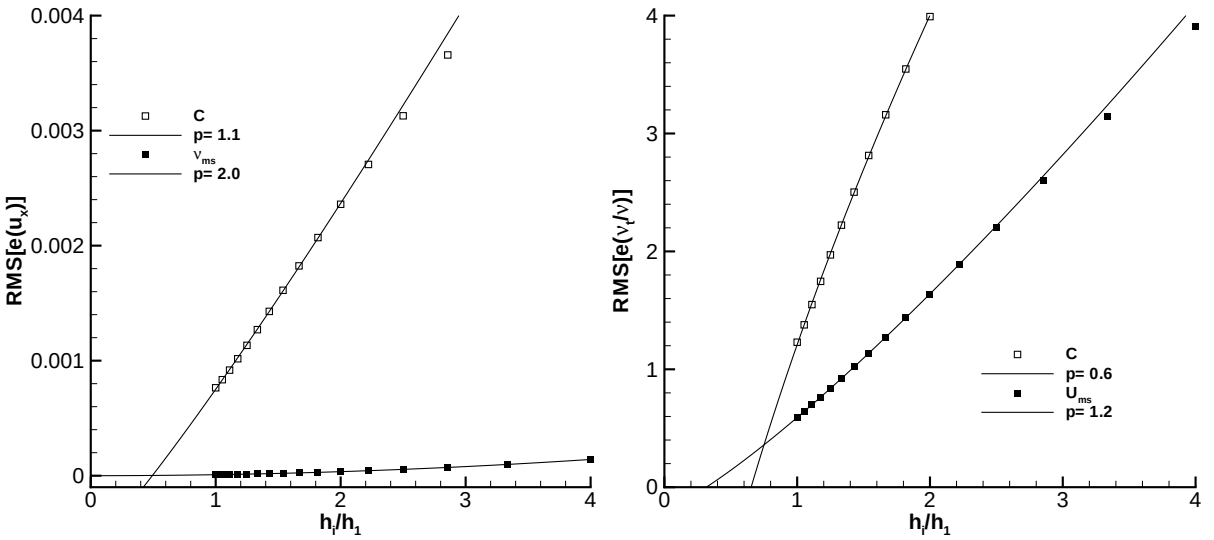

Figure 4: Convergence of the root mean square of the error of the horizontal velocity component, u_x (left), and of the eddy-viscosity, ν_t (right), as a function of the grid refinement ratio, h_i/h_1. MS for the one-equation turbulence model of Spalart & Allmaras and Menter.

calculation of the velocity and pressure fields with the manufactured eddy-viscosity, ν_{ms}; calculation of the complete flow field, C.

The results show that in the calculation of the velocity and pressure fields with the manufactured eddy-viscosity u_x exhibits the theoretical order of the method with the data clearly in the so-called 'asymptotic range'. On the other hand, the convergence of the eddy-viscosity with the manufactured velocity field exhibits an order of accuracy close to 1 and a non-vanishing error for the extrapolation to cell size zero. The problems obtained in the solution of the turbulence model transport equation are reflected in the u_x convergence for the complete flow field calculation.

The convergence difficulties illustrated in figure 4 are caused by the dependence of the dependent variable of the turbulence model, $\tilde{\nu}$, on the fourth power of the distance to the wall[19]. With the present second-order accurate method, there is an oscillation in the $\tilde{\nu}$ (and consequently ν_t) profiles at the near-bottom region, which disappears very slowly with the grid refinement[19]. This means that the convergence properties illustrated in figure 4 for the RMS of the error are not representative of the convergence of the flow field in the complete computational domain. Furthermore, in the Spalart & Allmaras model, ν_t is obtained multiplying $\tilde{\nu}$ by a damping function, f_{v1}, which is a non-linear function of $\tilde{\nu}$. Therefore, in the regions where f_{v1} is active the convergence of ν_t and $\tilde{\nu}$ may not be the same.

Figure 5 presents the convergence of the local error of u_x and ν_t for the three exercises illustrated in figure 4 at $x = 0.75$, $y = 0.013$, which is a location that coincides with a grid node for all 16 grids of the grid set. The data plotted in figure 5 exhibit several interesting features:

- The calculations involving the solution of the turbulence model transport equations

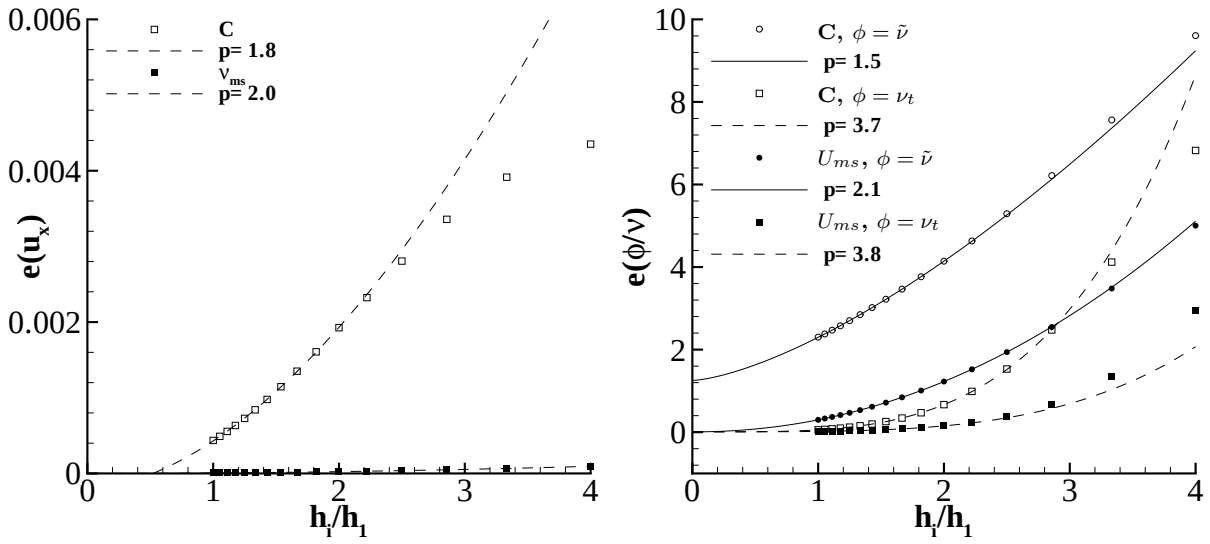

Figure 5: Convergence of the error of the horizontal velocity component, u_x, and of the eddy-viscosity, ν_t, as a function of the grid refinement ratio, h_i/h_1, at $x = 0.75$, $y = 0.013$. MS for the one-equation turbulence model of Spalart & Allmaras and Menter.

present local convergence properties significantly different from the ones obtained for the RMS of the error.

- The eddy-viscosity and the dependent variable of the model do not present the same convergence properties. There is a significant effect of the damping function, f_{v1}, which causes an artificially high level of the observed order of accuracy of ν_t.

- The calculation performed with the complete flow field shows a significant influence of the eddy-viscosity in the u_x convergence and vice-versa. The error of u_x is one order of magnitude larger than in the ν_{ms} calculations and the data do not appear to be in the so-called asymptotic range. On the other hand, the $\tilde{\nu}$ convergence of the complete flow field calculations presents an inconsistent extrapolation to cell size zero, which does not appear in the U_{ms} results.

5 FINAL REMARKS

We have discussed the application of the Method of the Manufactured Solutions (MMS) for Code Verification in incompressible, turbulent flows. Although the MMS is a purely mathematical exercise, it may not be straightforward to manufacture all the turbulence quantities involved in several of the most popular eddy-viscosity models. The existence of damping functions and/or blending functions including non-linear equations and undefined derivatives is problematic for the application of the MMS. Nevertheless, the MMS is almost a mandatory choice for Code Verification when eddy-viscosity turbulence models are involved, because there are no analytical solutions available.

The example presented in this paper shows the versatility of the approach which allows different exercises for a given flow solver. One can solve for the flow field with the manufactured eddy-viscosity field held fixed or vice-versa, i.e. solve the turbulence quantities transport equations with the velocity field fixed by the manufactured solution. Although we have not illustrated it in the present paper, it is even possible to go a step further and freeze any number of individual terms of the transport equations by taking them from the manufactured solution. Thus, it is possible to find the origin of any problem and the source of difficulties with the numerical convergence of the flow solution.

The results presented in this paper show that the solution of the continuity and momentum equations with a prescribed eddy-viscosity field is important, but not representative of the convergence properties obtained with the turbulence model active. In fact, the present data suggest that it is likely that the numerical properties of the transport equations of the turbulence models will be a disturbing factor in error estimation for complex turbulence flows.

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