NUMERICAL ANALYSIS OF THE MODELING AND NUMERICAL UNCERTAINTIES IN LARGE EDDY SIMULATION USING UPWIND-BIASED NUMERICAL SCHEMES

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INTRODUCTION

Accurate LES simulations can only be achieved if the numerical contamination of the smaller retained flow structures is taken into account as well as the subgrid parameterization (Geurts and Fröhlich, 2002). The interaction of the numerical and the modeling error complicates quality assessment procedures or uncertainty estimators of LES even further. This topic has recently been discussed in the literature (Celik et al., 2005; Chow and Moin, 2003; Geurts and Fröhlich, 2002; Klein, 2005; Kravchenko and Moin, 1997; Meyers et al., 2003; Hoffman, 2004). Klein (2005) proposed to evaluate the numerical as well as the modeling error using an approach based on Richardson extrapolation, where it is assumed that the modeling error scales like a power law.

Recently this method has been applied to several flow cases, like channel and free-shear flows and so far very encouraging results have been obtained using 2nd order CDS as discretization scheme. However, most commercial solvers able to handle complex geometries are not strictly second order accurate and often they are based on upwind biased schemes. Therefore it is extremely important to assess the applicability of the method to these schemes. The focus of this work is to investigate the method using a more diffusive numerical scheme, e.g. QUICK (Quadratic Interpolation for Convective Kinematics). As the model equations presented by Klein (2005) allow to distinguish between modeling and numerical uncertainty, their interaction can be studied, also with respect to the error components obtained by the CDS calculations.

The next section will introduce the method, originally proposed by Klein (2005) and recently extended by Freitag and Klein (2006). Subsequently the scaling exponent will be evaluated which is a necessary requirement to solve the model equations. The method will be applied to a strongly swirling, recirculating flow and to a channel flow.

CONFIGURATIONS AND NUMERICAL TECHNIQUE

Two configurations will be studied within this contribution. The first configuration will be the well known channel configuration at a Reynolds number of $Re_\tau = 395$, based on the wall friction velocity, cf. Moser et al. (1999). The extension of the computational domain in axial x, spanwise y and vertical z direction is $12\delta \times 6\delta \times 2\delta$ similar to Kim et al. (1987), where δ is the channel half width. The computational domain is resolved with $128 \times 64 \times 32$ grid points. All boundary conditions and further details are given in Klein (2005); Freitag and Klein (2006).

The second configuration will be a strongly swirled isothermal flow case where experimental data and corresponding DNS data can be taken from the literature (Schneider et al., 2005; Freitag and Klein, 2005; Freitag et al., 2006). The experimental setup consists of a movable block type swirler which feeds an annulus from where the airflow enters the measurement section at ambient pressure and temperature. The Reynolds number (5000) is calculated from the bulk velocity and the bluff-body diameter. The geometrical swirl number is set to S=0.75. The extension of the computational domain in axial x, and radial r direction is $12D\times 8D$. The computational domain is resolved with $360 \times 128 \times 120$ grid points.

The governing equations for the flow configurations investigated are the conservation equations of mass and momentum for an incompressible Newtonian Fluid in their instantaneous, local form. The equations are solved by using a finite volume technique. All variables are located on a staggered Cartesian grid for the channel flow and an a cylindrical mesh for the swirl flow respectively. For spatial discretization of convection upwind biased schemes, namely a QUICK scheme, are used, while temporal discretization is accomplished using an explicit third order Runge-Kutta-method. Former results using a 2nd order CDS scheme will be used as reference for a quantification of the influence coming from the numerical scheme (Freitag and Klein, 2006). The Poisson equation is inverted by using a direct fast elliptic solver.

THEORETICAL DERIVATIONS

A common way to assess the quality of CFD simulations in the context of RANS is to perform grid refinement studies, based on variants of the Richardson extrapolation (Roache, 1998). This is to some extent problematic for implicit filtering since both, numerical and modeling contribution scale with the filter width. In addition, the modeling and numerical errors interact which will question the terminology of a grid independent LES. Strictly speaking, implicit LES is only the solution to a set of differential equations on the discretized grid, since the model contribution depends on the grid spacing. This makes the verification of LES based on grid refinement studies difficult.

Ways out for this dilemma have been collected recently in the review of Celik et al. (2006). Klein (2005) studied the sensitivity of the simulation results on the modeling and numerical error contributions separately. The method requires two additional simulations to assess the results of the initial LES: One will be a grid variation and the second uses a modified model contribution. Intuitively it is clear that from such a model variation, the influence of the sgs parameterization can be assessed at least qualitatively.

To illustrate the idea, it is assumed in the following that the contribution from the numerical error (n) and the contribution from the model term (m) are given by the right hand side of a Taylor expansion (1) and that the leading order terms of both contributions are independent. The reasoning behind the structure of the model equation is given in the work of Klein (2005) in great detail and will not be repeated here.

The set of equations where u denotes the exact solution, u_1 the standard LES solution, u_2 the LES solution with a modified model contribution, and u_3 the solution obtained on a coarse grid, can be expressed in the following form,

$$u - u_1 = c_n h^n + c_m h^m \quad (1)$$

$$u - u_2 = c_n h^n + \alpha c_m h^m \quad (2)$$

$$u - u_3 = c_n(\beta h)^n + c_m(\beta h)^m. \quad (3)$$

Equation (2) is the equivalent of a simulation where the model contribution was modified by a certain factor α. Coarsening or refining a grid by a factor of β, where e.g. grid halving is equivalent to $\beta = 2$ leads to equation (3). The idea that the modeling error scales like a power of Δ originates in the pioneering work of Lilly (1967). The exact scaling can be obtained by equating the mean square of strain $\overline{S}$ and its spectrum. The scaling for the resolved stresses can then be deduced as $\overline{S} \sim \Delta^{-2/3}$ (Pope, 2000; Sagaut, 1998).

Combining equations (1)-(3) the error contribution can be split into model (4) and numerical error (5). The total error is the sum of both (see equation (6)).

$$(u_2 - u_1)/(1-\alpha) = c_m h^m \quad (4)$$

$$\frac{(u_3 - u_1) - (u_2 - u_1)(1-\beta^m)/(1-\alpha)}{1-\beta^n} = c_n h^n \quad (5)$$

$$\frac{u_3 - u_1 + (u_2 - u_1)(\beta^m - \beta^n)\ (1-\alpha)}{1-\beta^n} = c_n h^n + c_m h^m \quad (6)$$

Labeling equation (4) as modeling error might be misleading since it does not represent the classical model error. Rather, it represents the uncertainty introduced through the model on the particular grid with respect to the DNS. A more conservative approach to estimate the error was presented in the work of Freitag and Klein (2006). They additionally introduced the triangle inequality, $|c_n h^n + c_m h^m| < |c_n h^n| + |c_m h^m|$, to prevent partial cancellation of the individual errors which might occur if they are of opposite sign. Therefore it is suggested to use the conservative variant presented in equation (7) to estimate the uncertainty.

$$\left|\frac{(u_2 - u_1)}{(1-\alpha)}\right| + \left|\frac{(u_3 - u_1) - (u_2 - u_1)\frac{(1-\beta^m)}{(1-\alpha)}}{1-\beta^n}\right| = |c_n h^n| + |c_m h^m| \quad (7)$$

Independent which of the two variants is chosen, the system of equations is under-determined, since only three equations were formulated for five unknowns (u, n, m, c_m, c_n). To keep the method feasible it is suggested to make an assumption for the scaling exponents, rather than expanding the system of equations.

The scaling of the numerical scheme is usually known to the user through the numerical accuracy of the specific code. A 2nd order CDS and a 3rd order QUICK scheme will be applied to the method. In combination with a 2nd order integration of the finite volume method the numerical scaling is assumed to be equal 2.

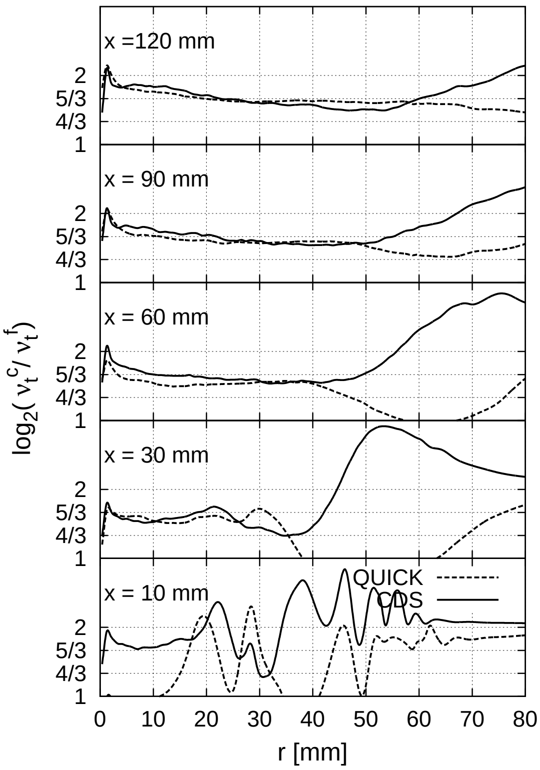

Figure 1: Logarithm of the ratio of the turbulent viscosities taken from simulations on two grids with a refinement ratio of two – ν_T^c corresponds to the coarse grid and ν_T^f to the fine grid, respectively.

The determination of the scaling exponent of the model term will be subject of the following section involving ideas already presented in Klein et al. (2006).

QUANTIFICATION OF THE SCALING EXPONENTS

Equation (1) assumes that the model error scales with the power of h. Using four sets of simulation results, Celik et al. (2005) determined the scaling exponent m to be approximately 2, i.e. a second order dissipation error. The theoretical dissipation error scales like $\Delta^{2/3}$ (Pope, 2000; Sagaut, 1998).

The Smagorinsky approach takes advantage of Prandtl's mixing length hypothesis (Prandtl, 1925) to model the eddy viscosity,

$$\tau_{ij}^{sgs} \approx 2\nu_T \widetilde{S_{ij}} \quad (8)$$

$$\nu_T = (C_s \triangle)^2 \sqrt{2\widetilde{S_{ij}}\widetilde{S_{ij}}} \quad (9)$$

Consistent with the observation $\tau_{ij} \sim \Delta^{2/3}$, the theoretical scaling for the eddy viscosity is $\nu_T \sim \Delta^{4/3}$ and $S_{ij} \sim \Delta^{-2/3}$. This will be easily checked a posteriori in a two grid study. At this point the procedure of Klein et al. (2006) is adopted where the scaling exponent was calculated through a comparison of the averaged turbulent viscosities of the calculation.

Figure 1 presents the log ratio of the turbulent viscosities on two different grids, coarsened by a factor of two. Results are presented for CDS and QUICK simulations of the complex swirling flow configuration at $Re = 5000$. As a general feature, the ratio of the turbulent viscosities is roughly constant in the regions of fully developed turbulence, but fluctuates in the shear layer and in the outer, laminar regions. For regions of fully developed turbulence the scaling for both, CDS and QUICK simulation, is almost identical. However at the outer radii, where the flow laminarizes m increases for the CDS and decrease using a QUICK scheme. This can be explained with different spreading angles of the simulation on the coarse and fine grid. Furthermore the spreading angle is influenced by the numerical scheme which leads to the different course of the curves.

From figure 1 it can be concluded that $\nu_T \sim \Delta^{5/3}$ seems to be a reasonable approximation. A calculation of the log ratio of the turbulent viscosity (9) for laminar flows will lead to $\log_2(\nu_T^c/\nu_T^f) = 2$ since S_{ij} will be identical on both grids. This will only hold true for the Smagorinsky model but not for its dynamical variant where the constant will be zero in laminar flow regions. Hence a range is spanned between $4/3 \ldots 5/3$, where the upper limit corresponds to moderate Reynolds numbers ($Re \approx \mathcal{O}(10^2 - 10^4)$ and the lower limit to high Reynolds numbers.

This implies that $\bar{S} \sim \Delta^{-2/3} \ldots \Delta^{-1/3}$ and hence $\tau_{ij} \sim \Delta^{2/3} \ldots \Delta^{4/3}$, i.e. $m = 2/3 \ldots 4/3$ which is within the expected range as explained above. The value $m = 4/3$ is used in the following section because of moderate Reynolds number flows.

APPLICATION TO THE SWIRLING FLOW

The error of the mean stream-wise velocity is plotted for one half of the domain in figure 2 showing both the predicted error (upper part) using the model equations (1)-(3) and the true error as difference between the DNS solution and the assessed LES (lower part). Even the color scaling is not identical in both plots, some key features can be identified. These are in detail an increasing error in the shear layers and a diminishing deviation from the ideal solution in the outer flow region, where the flow is supposed to be almost laminar. Note that the solution of the coarse grid and also the DNS solution was interpolated onto the LES mesh, hence the lower part of the figure appears to be much smoother compared to the predicted error on the upper half of the picture.

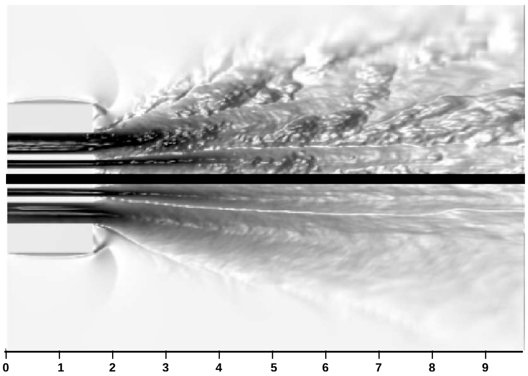

Figure 2: Contour-plot of the error-distribution for the swirling flow. Predicted Error (upper part) and true error as deviation from the corresponding DNS data (lower part).

A more quantitative comparison is presented in figure 3 where the results of the procedure given by equation (7) are compared to the real error calculated as absolute value of the difference to the DNS data. The overall course for the mean velocity deviation is predicted quite precise, especially at $x = 30$mm and further downstream. However, a significant over-prediction can be monitored close to the axis at $x = 10$mm and $x = 60$mm. Inspecting the particular error contributions at figure 4 (top) it becomes obvious that the conservatism of the triangle inequality leads to this over-prediction. Otherwise the opposite sign of the numerical and modeling error contribution would cancel the total error at these regions.

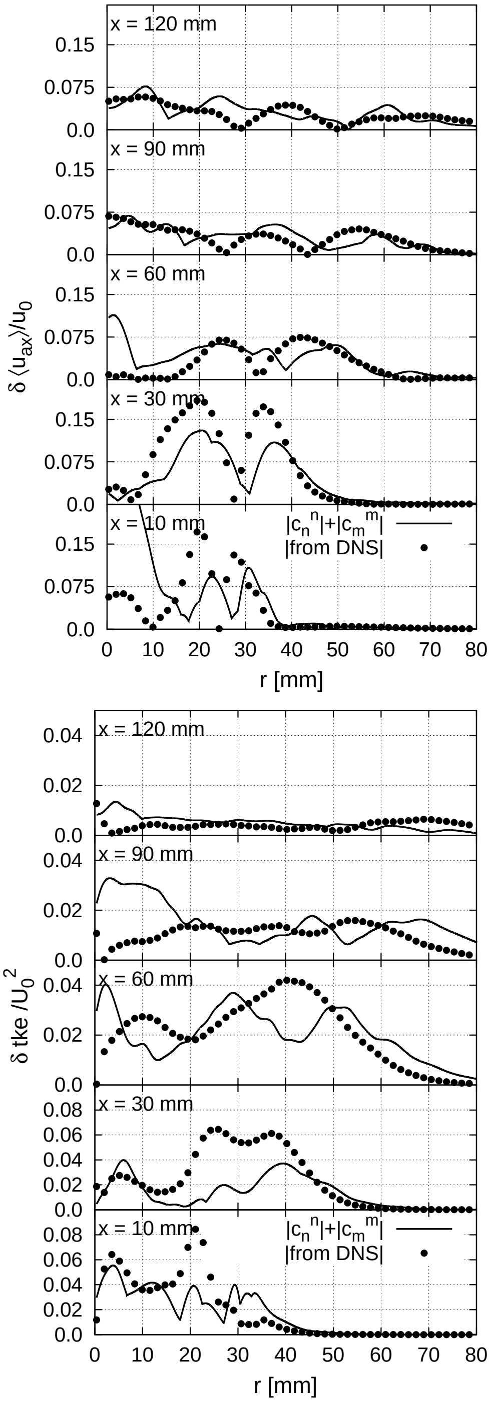

Figure 3: Application of the procedure given in equation (7) to the QUICK simulation to estimate the deviation for the mean stream-wise velocity (top) and the tke (bottom).

Nevertheless the authors recommend the use of the modified procedure, presented in Freitag and Klein (2006), due to the conservatism of this variant. A similar well behavior of the method can be found for the assessment of the turbulent kinetic energy (tke), see figure 3 (bottom). Nevertheless, some deviations can be identified for the maximum values at $x = 10\text{mm}$, $x = 30\text{mm}$ and $x = 60\text{mm}$. The general trend and the absolute level of the simulation error is captured, even not as perfect as the method predicted the error using a 2nd order CDS as convective discretization scheme, see Freitag and Klein (2006).

Discussion of the Separated Error Contributions

The individual error distribution can be calculated with the help of equations (4) - (6). Results of the QUICK calculations are presented at figure 4, corresponding CDS results are plotted at figure 5. A comparison of the modeling and the numerical error for the QUICK simulation yields that the larger error contribution comes from the model term and not from the numerical terms. This unexpected fact can be interpreted as follows. Local oscillations of the CDS scheme will be compensated by a higher turbulent diffusivity ν_t. The numerical error of the less dispersive QUICK scheme behaves like an additional diffusion hence the turbulent diffusivity ν_t needs no further increase.

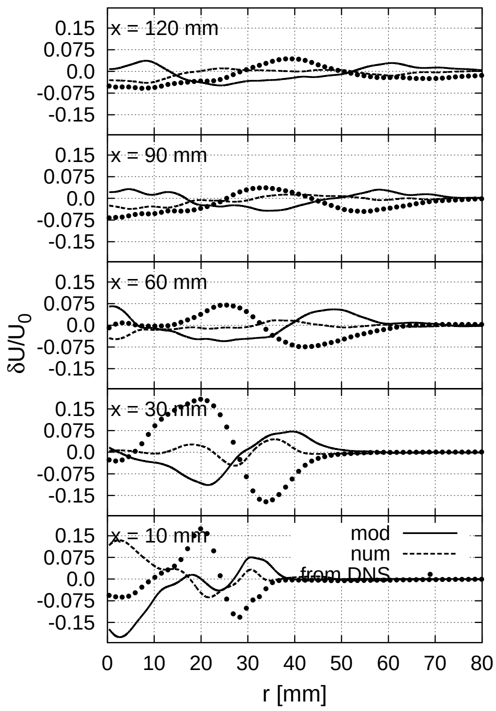

Figure 4: Distribution of the individual error contributions for the QUICK prediction.

An interesting feature for the CDS calculation is the correlation between the real error and the modeling contribution. Another significant observation for the CDS calculation is the similar magnitude of the two error contributions together with the opposite sign, so roughly $c_n h^n = -c_m h^m$ is given. Such trends can not be identified for the QUICK-LES besides very few exceptions. Hence the relation and the interaction between numerical and modeling error seems to be less connected, here.

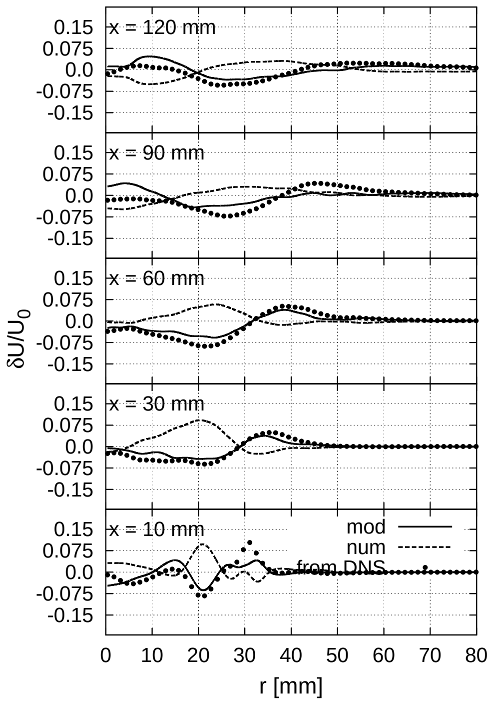

Figure 5: Distribution of the individual error contributions for the CDS calculation.

The overall deviation from the DNS data increases for the QUICK simulation especially at the core of the jet ($x = 10...30\text{mm}$) whereas the prediction is of similar quality further downstream. These deviations are visible for the kinetic energy where the QUICK scheme predicts overall higher values than the DNS and the CDS simulation (figure 6).

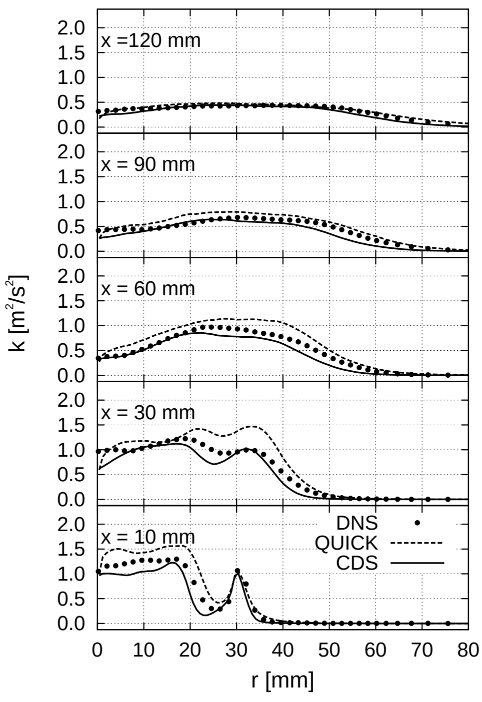

Figure 6: Radial profiles of the resolved turbulent kinetic energy, given at different axial heights.

This is to some extent surprising since the higher diffusivity of the numerical scheme should reduce the level of predicted kinetic energy. A possible explanation refers to the existence of the highly energetic coherent structure. A visualization of the PVC using pressure iso-levels, not shown here, reveals that the extent of the structure is larger for the QUICK simulation. Furthermore it is known from earlier studies (Freitag and Klein, 2005) that the bulk of the kinetic energy is directly related to the coherent motion and not to turbulent fluctuations. Therefore an over-prediction of the kinetic energy is explicable despite the usage of a more diffusive scheme.

APPLICATION TO THE CHANNEL FLOW

Task of this section is to incorporate the method to analyze the result of a simulation using the QUICK discretization for a channel flow at moderate Reynolds number, $Re_\tau = 395$.

The simulation results are compared to DNS data and former CDS calculations (Klein, 2005). Presented in figure 7 are mean values (top) and corresponding fluctuations (bottom) of the stream-wise velocity component. The solid and dashed lines belong to the results of the CDS calculations and the lines with points involving the same line style depict the results of the corresponding QUICK simulations. For the simulation using a Smagorinsky constant of $C_S = 0.1$ the results differ only slightly, however for a reduced model constant $C_S = 0.05$ the QUICK simulation notedly overshoots the DNS results. Obviously the QUICK simulation possesses a high sensitivity to the constant C_s whereas the CDS results are more independent from C_s.

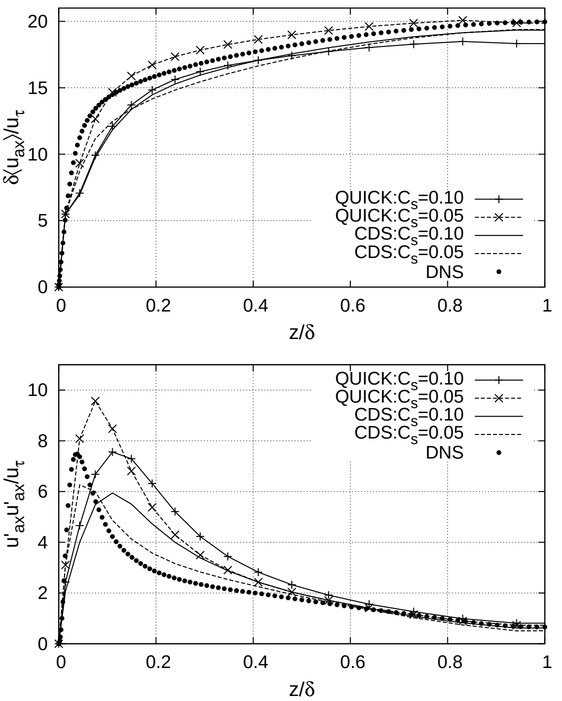

Figure 7: LES results using different Smagorinsky constants and convective schemes. The upper figure illustrates the mean stream-wise component, whereas the lower picture presents the prediction of the corresponding fluctuations.

The superiority of the CDS scheme becomes more perspicuous by inspecting the fluctuations of the stream-wise velocity components, at the lower part of figure 7. For a reduced model constant $C_S = 0.05$ the CDS results yield a reasonable close agreement to the DNS but both QUICK simulations fail to predict the position and the shape of the shear layer fluctuations. Even though a reduction of C_s leads to a steepening of the shear layer, the result deviates considerably from the DNS. Noticeable, the QUICK predicts generally higher absolute values for the wall shear layer. Flow visualizations reveal that the turbulent structures are much larger for the more diffusive scheme which leads directly to a higher fluctuation level.

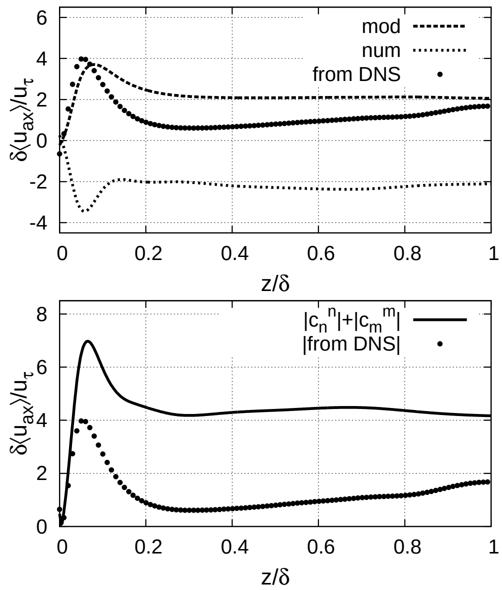

Figure 8: Application of the method given in equations (4) - (6) (top) and the conservative variant of (7) (bottom). Predictions for the mean of the stream-wise velocity component are presented.

Despite the fact that a simple comparison with the corresponding CDS-LES calculation evinces already a reduced prediction quality of the QUICK-LES, the methods of Klein (2005) and Freitag and Klein (2006) will be applied, also. Again the focus is put on the mean (figure 8) and fluctuations (figure 8) of the stream-wise velocity. The upper figures illustrate the particular contributions of equation (5), and the lower figures present results using the conservative approach, given in equation (7).

Compared to the results obtained with a CDS calculation (Freitag and Klein, 2006) the model behaves less optimal for upwind biased numerical schemes. Even though the course of the error contribution is predicted well the absolute value differs. The summation of the error from the model contribution and the numerical error yields a strong under-prediction for the total error, calculated as difference to DNS data. This is primarily due to the fact that the magnitude of both errors are almost identical over the entire range of the channel. In combination with an alternating sign this leads to a cancellation through the summation of the segregated error contribution. This is also the reason why the rectified conservative method over-predicts the absolute error (figure 8 top).

Improvement of the results can naturally be achieved by a modification of m and n, however we like to put this aside, to keep the universality of the procedure. The agreement between the error for the fluctuations and the deviation from the DNS data is similar to the mean quantity. Again the basic features i.e. the strong discrepancies at the shear layer

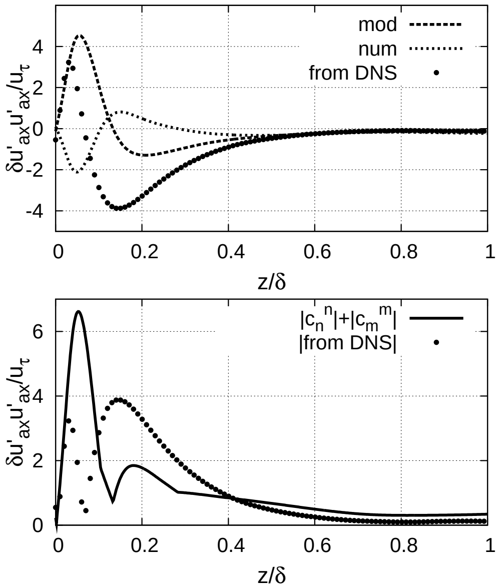

Figure 9: Application of the method given in equations (4) - (6) (top) and the conservative variant of (7) (bottom). Predictions for the fluctuations of the stream-wise velocity component are presented.

are captured, but the magnitude is predicted less accurate.

CONCLUSIONS AND OUTLOOK

A method to assess the quality of LES has been applied to a free swirling flow and a channel flow, using different numerical schemes, i.e. 2nd order CDS and QUICK schemes. The positive side-effect of the method is the separate availability of the numerical and the modeling error distribution.

Concluding it can be stated that the method works slightly worse for a more diffusive numerical scheme compared to former CDS predictions. The reason for this deviating behavior might be the fact that a mixed discretization has been used, i.e. a QUICK scheme for the convective terms and a CDS scheme for the diffusive terms. However the method displayed once more that a simplification to an error predictor relying only on a single grid refinement is problematic since the errors interact and more drastically they appear to be of similar magnitude. A comparison between the CDS and the QUICK results yields that the difference is quite strong for a wall bounded flow at moderate Reynolds number and is almost invisible for an unconfined swirling flow.

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