The Effect of the DNS Data Averaging Time on the Accuracy of RANS-DNS Simulations

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Statistical data obtained from direct numerical simulations (DNS) are often used as reference data for validating turbulence models. Thus, accuracy of the DNS data itself is of particular importance for understanding the potential error in Reynolds-averaged Navier-Stokes (RANS) simulations. Recent studies demonstrate that when the DNS data is used to represent budget terms in the RANS equations, simulations of wall-bounded turbulent flows conducted with such equations (herein referred to as RANS-DNS simulations) produce unphysical results. The current paper analyzes the contribution that convergence of DNS statistics makes to this discrepancy. The Reynolds stresses and budget terms in the RANS equations are collected in a fully developed channel flow ($Re_\tau = 392$) at increasing sample sizes and analyzed using the RANS-DNS simulation. The results demonstrate that statistical convergence is not the only contributing factor to the spurious RANS-DNS results, and further study is required.

Nomenclature

U	=	mean flow velocity in the streamwise direction
U_∞	=	free stream velocity
U^+	=	U / u_τ
P	=	mean flow pressure
u, v, w	=	turbulent velocity fluctuations in streamwise, normal-to-wall, and spanwise directions
u_i	=	turbulent velocity fluctuation in the i-direction
u_τ	=	friction velocity
h	=	half-channel width
t	=	time
t_n	=	averaging time of DNS data
δ	=	boundary layer thickness
θ	=	boundary layer momentum thickness
ν	=	kinematic viscosity

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Re_τ = Reynolds number, $\delta u_\tau / \nu$
Re_θ = Reynolds number, $\theta U_\infty / \nu$
y_+ = $y u_\tau / \nu$
<…> = ensemble averaging
$< u_i u_j >^+$ = $< u_i u_j > / u_\tau^2$

I. Introduction

THE availability of accurate reference data is essential for the development and validation of turbulence models. Such data are typically obtained from experiments. However, difficulties associated with experimental measurements and the cost of experiments limit available datasets. Direct numerical simulation (DNS) on the other hand can produce all statistics required for model validation.

DNS data are collected in simpler flow geometries and at lower Reynolds numbers than observed in aerospace applications. Nevertheless, validation of a turbulence model against DNS data provides a valuable insight into the model predictive capabilities, because a successful model is expected to perform in a wide range of Reynolds numbers and flow geometries. If a model fails to deliver accurate results in flows with simpler physics, there is no reason to expect for the model to provide such results in more complex flows.

The accuracy of data used as a reference should be quantified. In DNS, the standard approach for estimating the accuracy of collected velocity moments, such as the Reynolds stresses, is to compare the orders of magnitude of residual balances (balance errors) with the values of individual terms in the corresponding Reynolds-averaged Navier-Stokes (RANS) equations[1]. The acceptable level of uncertainty in the collected Reynolds stresses is determined by a subjective judgment and is strongly influenced by the cost of computations.

More rigorous procedures for evaluating the accuracy of statistical data collected from DNS were recently proposed[2,3]. In Ref. 2, the standard procedure for evaluating the order of magnitude of the budget balance errors is complimented with an estimate of the statistical errors. A Bayesian extension of Richardson extrapolation is used in Ref. 3. The procedures were applied to collect statistics in a zero-pressure-gradient boundary layer over a flat plate[4] and in a planar fully-developed channel flow[5], respectively. Both procedures are complex to implement and are not universal.

A new approach to quantifying uncertainty in DNS statistics that utilizes the self-consistency of RANS equations was developed in our group[6,7]. In this approach computed statistics from DNS are used to solve the RANS equations, and their solutions are compared back with the DNS data for velocity moments. Hereafter, such computations are called RANS-DNS simulations. The procedure is amenable to any flow geometry and straightforward to implement.

RANS-DNS simulations[6-8] conducted in planar wall-bounded turbulent flows such as a fully-developed channel flow and a zero-pressure-gradient boundary layer over a flat plate, with the DNS data from Refs. 4, 5, and 9 demonstrated that neither the standard approach[1] used in Ref. 9, nor recent advances[2,3] in evaluating the DNS data accuracy guarantee the data accuracy to be sufficient for generating RANS-DNS solutions in agreement with the DNS profiles for velocity moments.

Several possible sources of error or inconsistency have been hypothesized to cause the observed discrepancies in the RANS-DNS approach, such as discretization error, systemic error in the DNS post-processing or RANS-DNS approach, etc. Many of these issues have been addressed in previous studies, however a primary question of whether DNS data are statistically converged, and what effect a lack of convergence may have on the results, is unresolved. This paper aims to address this question.

RANS-DNS simulations are conducted in a planar fully-developed incompressible turbulent flow in a channel at $Re_\tau = 392$ using the open-source OpenFOAM solver[10] modified and validated[7] for such simulations. DNS budgets for the Reynolds stresses used in RANS-DNS simulations are obtained from DNS performed using a pseudo-spectral (Fourier/Chebyshev-τ) method[11]. Statistics are collected for an increasing number of statistical samples.

The paper begins with a review of both the DNS methodology and case description, followed by an overview of the RANS-DNS approach. Results of the study are presented next, in the form of RANS-DNS solutions and analysis of the convergence trends in the DNS data. Finally, some areas of future study based on the analysis are presented.

II. DNS methodology

DNS in a fully-developed channel flow is performed at the Reynolds number $Re_\tau = 392$ based on the friction velocity. This corresponds to the Reynolds numbers of 13,750 and 7,910 based on the bulk and centerline mean velocities, respectively. The Reynolds number is large enough to sustain a well-defined inertial sublayer, while still being computationally expedient to collect large number of samples. The incompressible Navier-Stokes equations are solved using a pseudo-spectral (Fourier/Chebyshev-τ) method. The parameters and procedures of this method are described in Ref. 11. The channel domain size of $2\pi h \times h \times \pi h$ is represented using $256 \times 193 \times 192$ spectral modes along the streamwise (*x*), wall-normal (*y*) and spanwise (*z*) directions respectively. As the first step, statistics are generated from each realization (i.e. a snapshot of the computational box, as shown in Fig. 1) and averaged along the streamwise-spanwise plane and 'folded' about the centerline, taking advantage of the flow symmetry. An ensemble of statistics generated from different realizations of the flow is used to average the statistics, thereby reducing the statistical error.

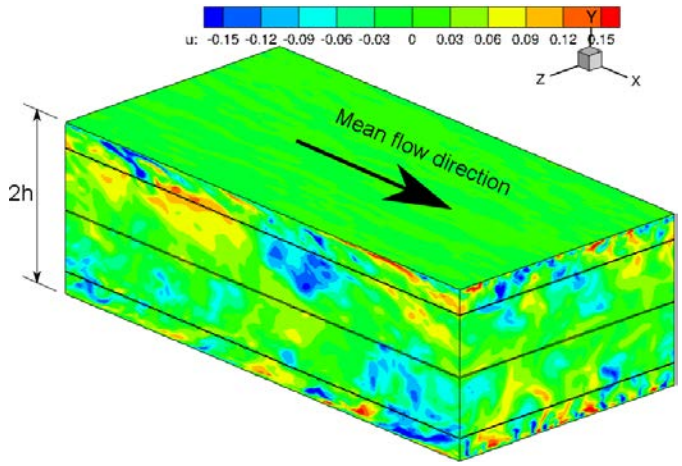

Figure 1. A realization of the fully-developed channel flow, colored by fluctuating streamwise (u^+) flow velocity.

In each realization, the mean flow velocity, *U(y)*, and pressure, *P(y)*, are evaluated from the 0^{th} mode of the velocity and pressure fields along the *x-z* plane. The fluctuating components are evaluated from the corresponding non-zero modes. Velocity and pressure values are stored at the same grid nodes, and their gradients are evaluated in the Fourier space. The statistical moments and their budgets are evaluated by building correlations in physical space,

$$< f >= \sum_x \sum_z f.$$

In Ref. 9, an ensemble set of 159 realizations was found sufficient to statically converge the Reynolds stresses and their budget terms. The successive realizations are spaced apart by two bulk flow-through times. In the current study, ensemble sets of 21, 50, 100, 200, 500 and 1000 realizations were generated, with the successive realizations being spaced apart by one bulk flow-though time to minimize computational resources, while retaining statistical "independence". By virtue of periodicity, gradients of statistics along the streamwise and spanwise directions are equal to zero, $\partial <.>/\partial x = \partial <.>/\partial z = 0$, thereby reducing the number of terms needed for the Reynolds stress budget evaluation. The dissipation term involves products of the velocity fluctuation gradients and hence, is sensitive to the errors in the gradients evaluation. It has been shown in section 4.2 of Ref. 9, that the grid spacing used is sufficient to resolve the dissipation term accurately both near the channel wall and at the channel centerline.

III. RANS-DNS simulations

In RANS-DNS simulations, the exact RANS equations are solved, with no modeling involved. All budget terms except for the molecular diffusion are substituted with the data collected from DNS for these terms. In this formulation all the equations are uncoupled so that there is no interdependency of their solutions. The solutions are compared with the DNS data for the corresponding velocity moments. The discrepancy between the RANS-DNS simulation solution and the DNS profile of the corresponding velocity moment serves as an indicator of the solution accuracy.

In the paper, the RANS equations are solved for the Reynolds stresses:

$$\frac{D < u_i u_j >}{Dt} = D_{ij}^M + D_{ij}^T + P_{ij} + \Pi_{ij} - \varepsilon_{ij} \quad , \tag{1}$$

in a planar fully-developed turbulent channel flow. The terms shown by blue on the right-hand side of (1) are those from DNS. They are molecular diffusion (D_{ij}^M), turbulent diffusion (D_{ij}^T), production (P_{ij}), velocity-pressure-gradient correlations (Π_{ij}), and the dissipation tensor (ε_{ij}), respectively. For the study, the general form of (1) is simplified under the assumptions of a statistically stationary fully-developed planar turbulent flow.

Previous results[6,7] obtained in a fully-developed channel flow demonstrated that simulations with equation (1) do not produce self-consistent results using the RANS-DNS approach. In other words, simulations of the RANS equations using DNS data as the closure model do not reproduce the DNS mean flow profiles (Fig. 2a). In the figure, DNS profiles of the Reynolds stresses are shown by symbols and RANS-DNS solutions by solid lines.

The results can be “corrected” by including an “error” correction Err_{ij} in (1):

$$\frac{D < u_i u_j >}{Dt} = D_{ij}^M + D_{ij}^T + P_{ij} + \Pi_{ij} - \varepsilon_{ij} - Err_{ij}\,, \qquad (2)$$

which represents the balance errors determined from DNS for each equation, and the contribution from terms which should be zero in a statistically converged planar flow simulation, but are nonetheless non-zero due to the finite averaging time. These results are presented in Fig. 2b for the current channel configuration.

The results in Fig. 2 demonstrate that inaccuracies in the DNS budgets used in RANS-DNS simulations are the dominant source of uncertainty in the simulation results, whereas uncertainties introduced by a numerical procedure employed for simulations have no recognizable effect. This makes the RANS-DNS simulations a plausible framework for quantifying the total uncertainty in statistical data collected from DNS.

The common perception is that the major source of uncertainty in DNS data is a finite number of decorrelated flow realizations used to collect statistics. That is, by increasing the averaging time (equivalently, sample size), the error in RANS-DNS simulations will be reduced, with their solutions tending towards the DNS profiles. This perception was utilized in Refs. 2 and 4, for example, when computing statistics in a zero-pressure-gradient boundary layer over a flat plate. In the RANS-DNS approach, this would imply convergence of RANS-DNS solutions to DNS profiles of corresponding Reynolds stresses. The current paper investigates whether this is indeed the case.

RANS-DNS simulations are conducted with equation (1) using the open-source OpenFOAM solver[10] that has already been validated for such purpose[7]. The *simpleFoam* application from the OpenFOAM 2.3.0 library[10] is used to solve the Reynolds stress transport equations with a Preconditioned Bi-Conjugate Gradient solver (*PBiCG*) and a Diagonal Incomplete LU (*DILU*) preconditioner. Table 1 provides a list of numerical schemes used to discretize the equations.

The pressure-gradient source term in the mean flow velocity equation is added by specifying the *pressureGradientExplicitSource* option in the *momentumSource* dictionary, placed in the *fvOptions* OpenFOAM file inside the *system* directory of a case under consideration. The applied pressure gradient is chosen to match the DNS results.

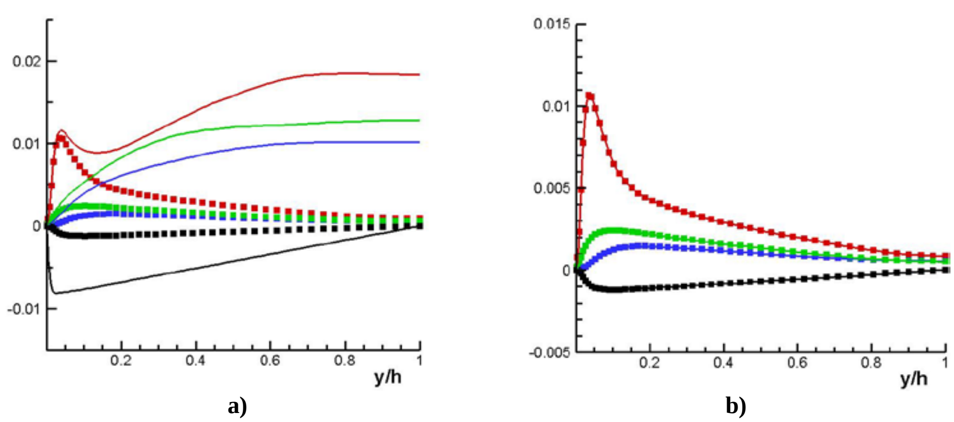

Figure 2. Reynolds stresses from RANS-DNS simulations conducted with (a) equation (1) and (b) equation (2) (solid lines) compared with their DNS profiles (symbols). Color scheme: red – $< u^2 >$, black – $< uv >$, blue – $< v^2 >$, green – $< w^2 >$.

Table 1. Numerical schemes as specified in the *fvSchemes* file.

Calculation	Keyword	Scheme
Gradient	*gradSchemes*	*Gauss linear*
Convection	*divSchemes*	*bounded Gauss linear*
Laplacian	*laplacianSchemes*	*Gauss linear corrected*
Time derivative	*timeScheme*	*steadyState*

The computational domain dimensions are $L_x \times L_y \times L_z = 0.1h \times 2h \times 0.1h$, with the channel half-width h being $1\ m$. Although the flow is fully developed, three-dimensional grids are required by OpenFOAM. The grid size is $N_x \times N_y \times N_z = 2 \times 193 \times 2$ nodes. The number of grid nodes (97) and their distribution in the wall-normal direction over the channel half-width are identical to that of the DNS data points in this direction. Initial values at the cell centers are interpolated from the DNS profiles available at the nodes. The cubic spline function is used when interpolation of the DNS data is required in this study.

Periodic (*cyclic*) boundary conditions are applied at the faces normal to the streamwise direction. Faces normal to the spanwise direction are defined as *empty*, which is a special type of boundary conditions used in OpenFOAM for two-dimensional problems. The remaining faces are defined as the type *wall*, where no-slip boundary conditions are applied to all flow parameters for which the equations are solved.

IV. Results

To analyze the effect of statistical convergence of DNS data used in RANS-DNS simulations on the accuracy of simulation results, simulations were conducted with the data averaged over seven different times: $t_1 = 3.92 \cdot 10^4$, $t_2 = 4.16 \cdot 10^4$, $t_3 = 4.57 \cdot 10^4$, $t_4 = 5.06 \cdot 10^4$, $t_5 = 5.4 \cdot 10^4$, $t_6 = 7.89 \cdot 10^4$, and $t_7 = 1.22 \cdot 10^5$. These times correspond to the following numbers of time steps: $4.72 \cdot 10^6$, $5.01 \cdot 10^6$, $5.51 \cdot 10^6$, $6.1 \cdot 10^6$, $6.51 \cdot 10^6$, $9.51 \cdot 10^6$, and $14.69 \cdot 10^6$.

Simulation results obtained with DNS data collected at t_2, t_3, t_5, t_6, and t_7 are shown in Fig. 3 by solid lines (green, blue, magenta, red, and black lines, respectively). As seen from the figure, the RANS-DNS solutions for the given Reynolds stress do not converge to their DNS profiles (symbols in the figure) at the times considered. It appears that the RANS-DNS simulations are converging towards an equipartition of energy across the channel width, "pinned" by the no-slip condition at the wall. This is clearly a non-physical result.

These results are at odds with the common point of view that statistical errors are the major contributor to uncertainties in statistics collected from DNS and therefore, the data accuracy can be improved by simply increasing the averaging time. In regard to RANS-DNS simulations, this would imply for their solutions to converge to DNS profiles of the corresponding Reynolds stresses. Notice that the uncertainty analysis of DNS data conducted in Ref. 3 in a fully-developed channel flow also demonstrated that large contributions from the discretization errors could not be completely ruled out for all collected statistics.

To illustrate the observed phenomenon in more detail, variations of the L_2-norm-based error:

$$Err_{L2} = ||f(t_n) - f(t_7)||, \tag{3}$$

of the statistical convergence are plotted in Fig. 4a, with f in (3) being the RANS-DNS solutions for the Reynolds stresses. The figure demonstrates that neither the RANS-DNS simulation results nor the DNS solutions (Fig. 4b) are converging monotonically with increasing the statistical sample size, and the convergence of $< v^2 >$ appears stalled. This implies the presence of a systematic error.

Notice that non-statistical nature of the DNS data convergence remains undetected when plotting DNS profiles of the Reynolds stresses itself (Fig. 5). They seem to converge rapidly with the profiles collected at different averaging times being very close to one another.

Results of RANS-DNS simulations shown in Figs. 3 and 4 call for in-depth investigation of the DNS data convergence and errors, as well as the RANS-DNS simulation process. Since the systematic error is present in DNS profiles of the Reynolds stresses, such an error should be expected in DNS budgets of the Reynolds stresses. Figures 6 -8 demonstrate convergence of individual terms in the Reynolds stress budgets. Except for the balance errors, dynamics of the individual budget term profiles is similar to that of the Reynolds stresses, that is, not very informative (Fig. 6). The profiles are very close to one another at different times, with some variation being observed near the channel wall. Plots of Err_{L2} (Fig. 7) reveal a more accurate picture. That is, none of the individual budget terms converges in a statistical sense. Thus, indeed, the systematic error is also present in DNS budgets of the Reynolds stresses.

Insight into the systematic error distribution in the direction normal to the channel wall can be obtained by plotting profiles of the balance errors in the budgets of different Reynolds stresses (Fig. 8). As seen from the figure, at later averaging times, t_6 and t_7, the balance errors do not change with time, revealing the systematic error distribution. The error maximum is clearly shifted towards the channel wall for all Reynolds stresses. This brings into question the effect of grid refinement on the DNS data accuracy. A finer grid with 192 nodes in a half channel

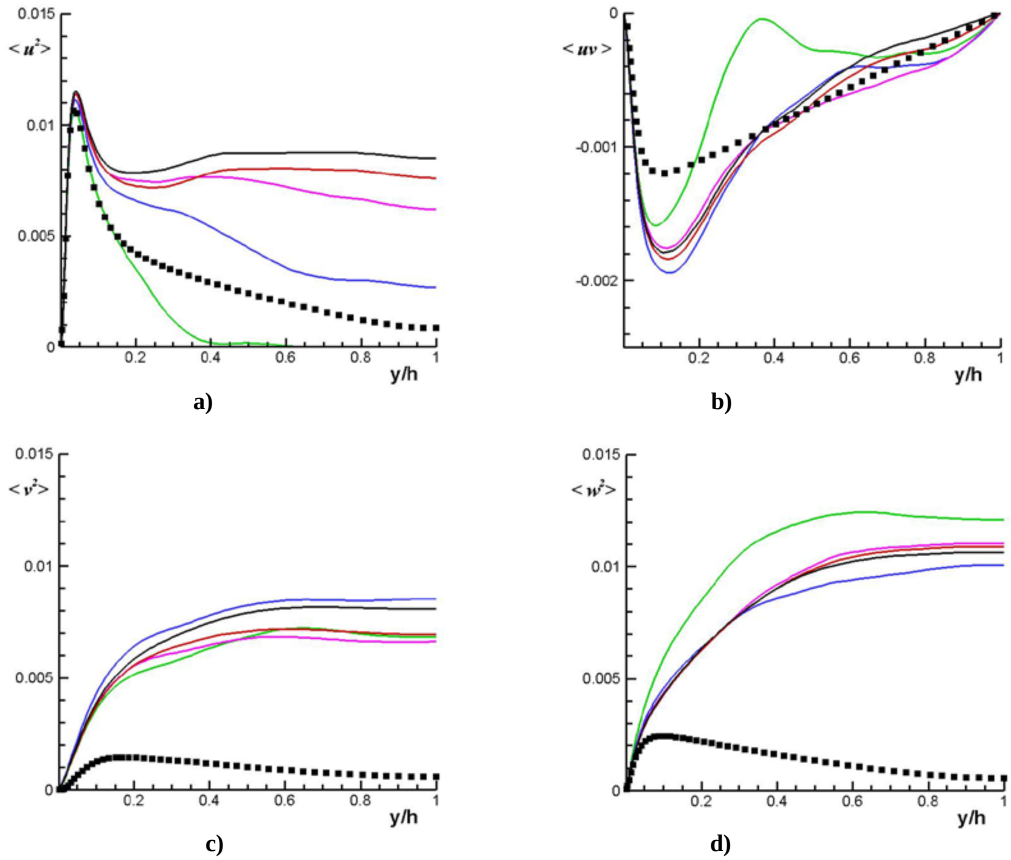

Figure 3. Reynolds stresses from RANS-DNS simulations (solid lines) obtained with DNS data (squares) in a fully-developed channel flow. Color scheme: green – t_2, blue – t_3, magenda – t_5, red – t_6, black – t_7.

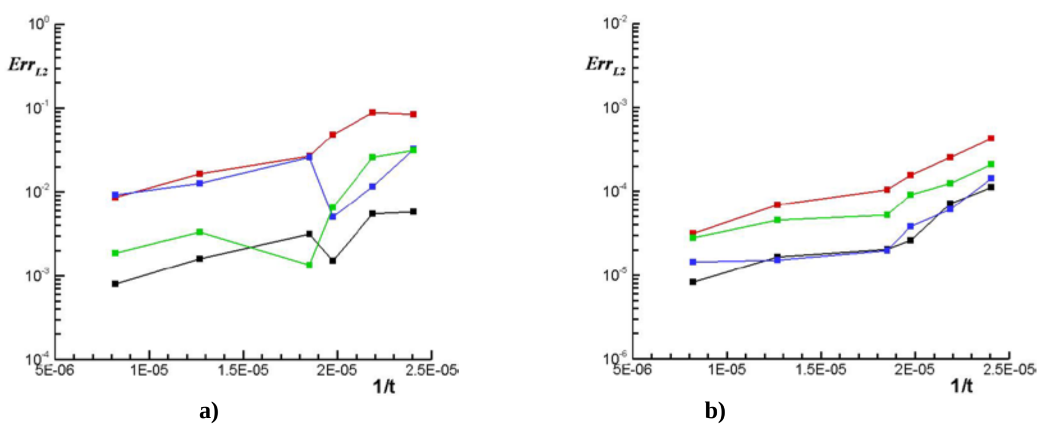

Figure 4. Err_{L2} for the Reynolds stresses in RANS-DNS simulations (a) and DNS profiles (b) with increasing the average time (from right to left). Color scheme as in Fig. 2.

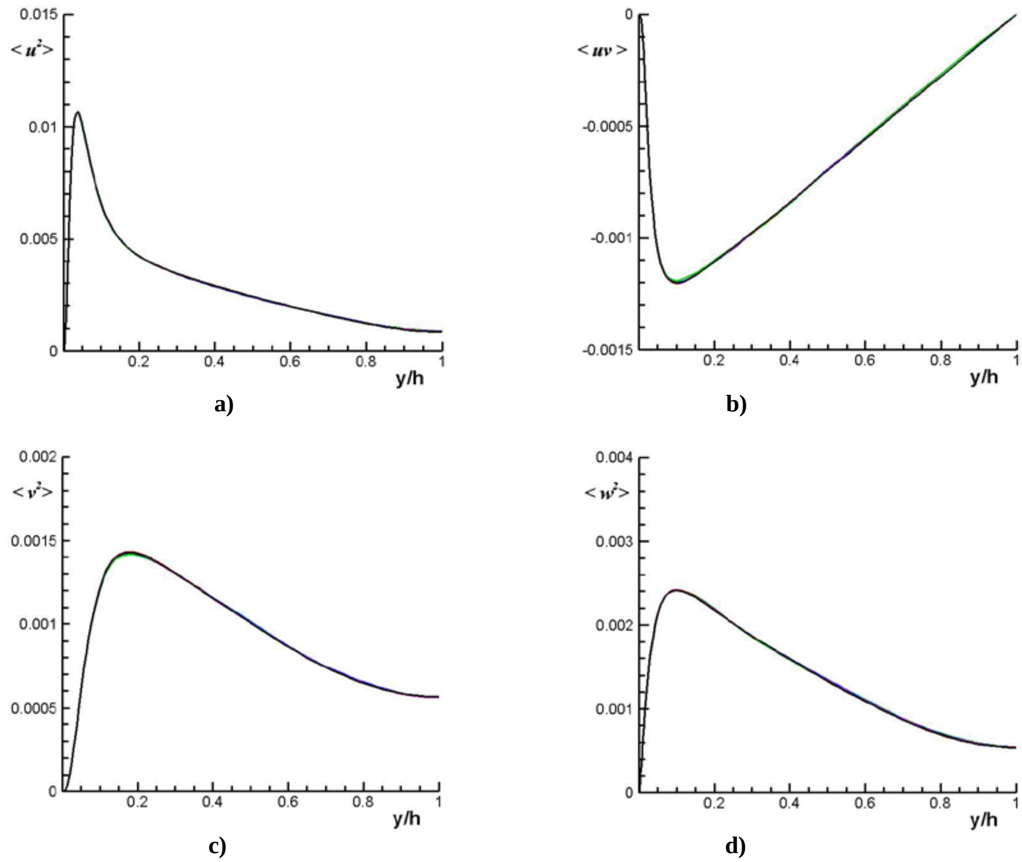

Figure 5. DNS profiles of the Reynolds stresses in a fully-developed channel flow at different averaging times. Notations as in Fig. 3.

width was used in Ref. 5 to compare with 97 nodes used in the current study. The grid spacing at the wall in the wall-normal direction is $\Delta y^+ = 0.019$ in Ref. 5 versus 0.1 in the current work, where $y^+ = yu_\tau/\nu$. In our separate study[8], we found that the results of RANS-DNS simulations conducted with DNS data[5] at comparable Reynolds number $Re_\tau = 550$ are significantly closer to DNS profiles of the Reynolds stresses than obtained in the current study (Fig. 3), which makes the grid resolution a plausible factor into the systematic error of DNS data. However, there are other differences in numerical procedures used in our study and in Ref. 5, which cannot be ruled out.
Contributions of all of them have to be investigated before any definite conclusion about the origin of the systematic error and its mitigation can be made.

Whereas a question about the systematic error origin in DNS data remains open at the moment, what is clear is that by simply increasing the averaging time, this error will not be reduced and as a result, neither will be reduced balance errors in DNS budgets and errors in DNS profiles of the Reynolds stresses to the degree sufficient for RANS-DNS solutions to converge to DNS profiles of the Reynolds stresses.

What we can estimate with the current data is the level of balance errors in DNS budgets at which such convergence may be expected. In Figure 9, absolute values of a ratio of balance errors to molecular diffusion

$$\left|Err_{\alpha\alpha}\right|'' = \left|Err_{\alpha\alpha}/D^M_{\alpha\alpha}\right|$$

in DNS budgets of different Reynolds stresses are shown at different averaging times. As seen from the figure, balance errors are of the same order of magnitude as molecular diffusion in the majority of the flowfield, exceeding it in some areas by the order of two. At later averaging times, no significant changes are observed in the ratio values. This explains why simulations with RANS equations are so sensitive to balance errors. The ratio can be used as a guide for an acceptable level of balance errors in the Reynolds stress budgets: it should be at least the order of magnitude smaller than molecular diffusion.

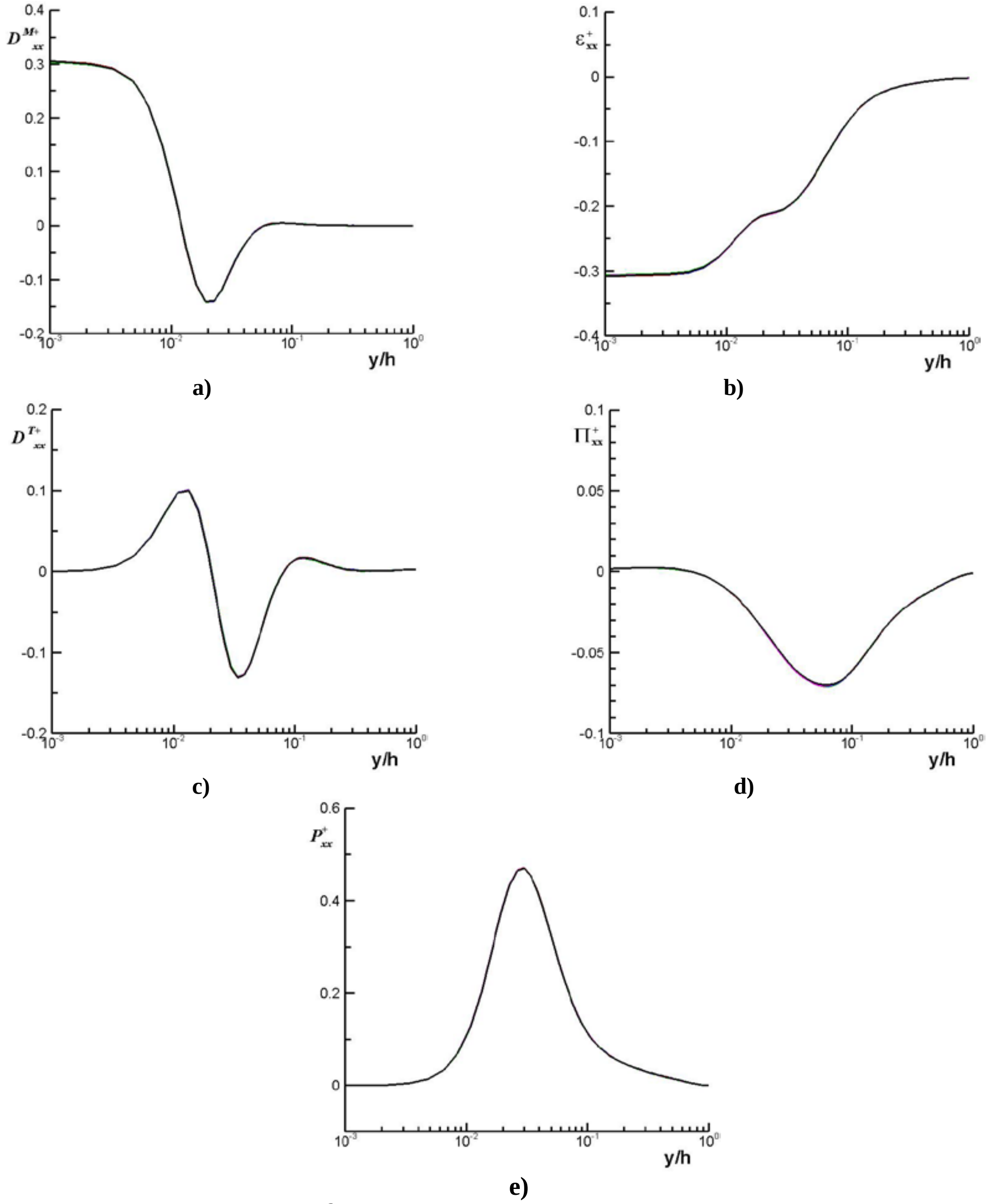

Figure 6. Terms in the DNS budget of $< u^2 >$ (non-dimensional in viscous units) at different average times: molecular diffusion (a), dissipation (b), turbulent diffusion (c), velocity/pressure-gradient correlations (d), production (e). Color scheme as in Fig. 3.

V. Future work

In the current paper, the effect of increasing the statistical sample size (equivalently, averaging time) used to collect statistics from DNS on the accuracy of RANS-DNS simulations conducted with the collected DNS statistics has been investigated. It was found that statistical errors in DNS data are reduced at earlier averaging times $t \leq 4.57 \cdot 10^4$, which corresponds to $5.51 \cdot 10^6$ time steps in the study. At later times, a presence of the systematic error in DNS data becomes apparent. Such an error cannot be reduced with increasing the averaging time and prevents convergence of RANS-DNS solutions to DNS profiles of the Reynolds stresses.

When turbulence models for individual terms in the RANS equations are calibrated against DNS budget terms with reduced statistical error, but the systematic error being present, results of simulation with such models will not reproduce the DNS profiles of the Reynolds stresses.

The paper also demonstrates that although DNS Reynolds stress profiles appear to converge rapidly, they do not converge in the statistical sense to the "true" solution, but to profiles with what appears to be a systematic error.

Currently, it is unclear in what degree the reduction of the systematic error will affect the Reynolds stress profiles. This has to be investigated in more detail.

The distribution of balance errors in the wall-normal direction was found to be non-uniform, with their maximum being shifted towards the channel wall for all Reynolds stresses. In this regard, the effect of grid refinement on the results of RANS-DNS simulation also has to be explored more carefully along with other potential contributors to the DNS data errors.

Future studies have also to focus on overall reduction of a ratio of balance errors to molecular diffusion, the smallest term in the Reynolds stress budgets. The ratio values in the current study were found to be unacceptably high (up to two orders of magnitude) that makes RANS-DNS simulations particularly sensitive to balance errrors in DNS data.

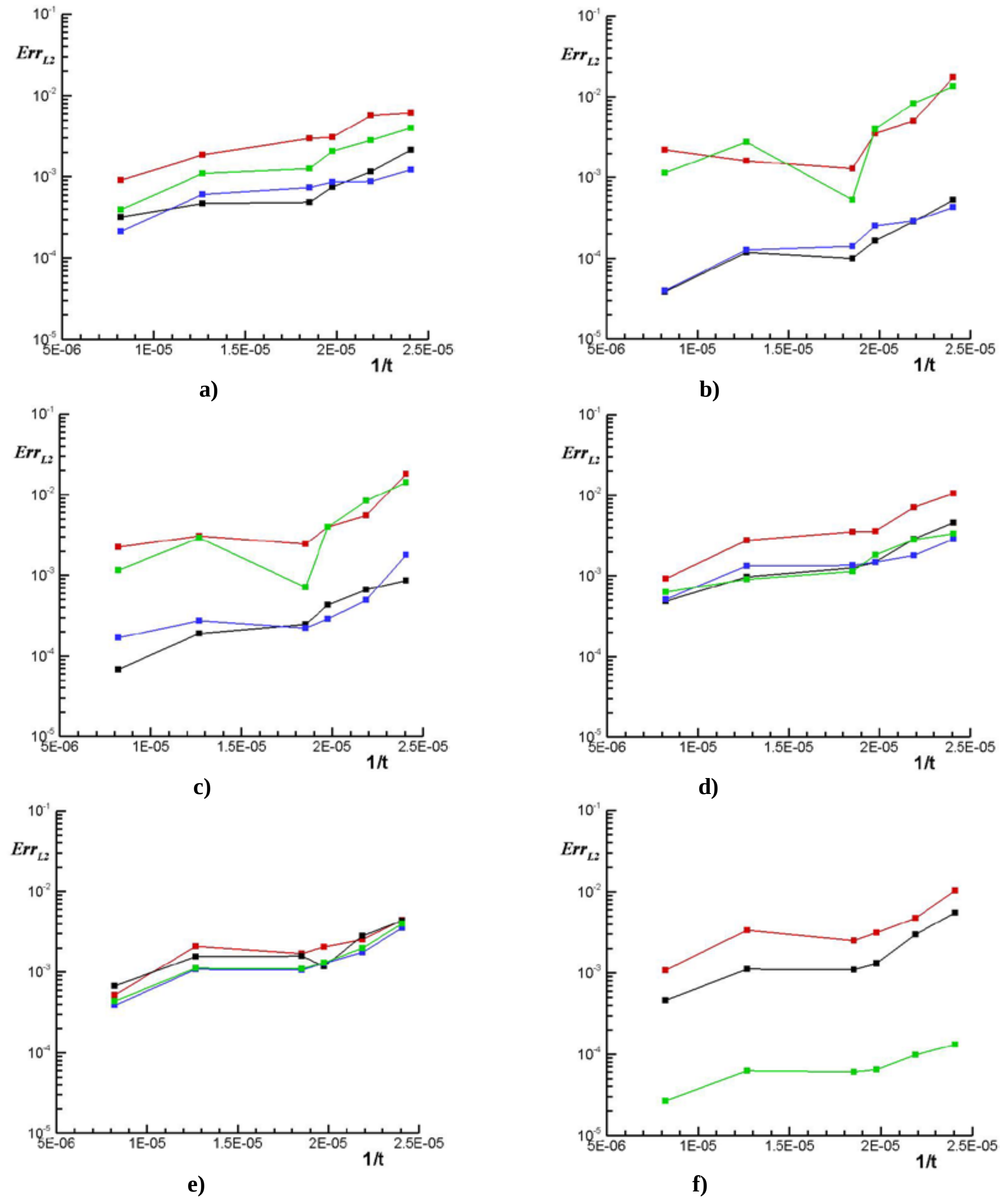

Figure 7. Err_{L2} of the terms in DNS budgets of the Reynolds stresses with increasing the average time (from right to left): balance errors (a), molecular diffusion (b), dissipation (c), turbulent diffusion (d), velocity/pressure-gradient correlations (e), production (f). Color scheme as in Fig. 2.

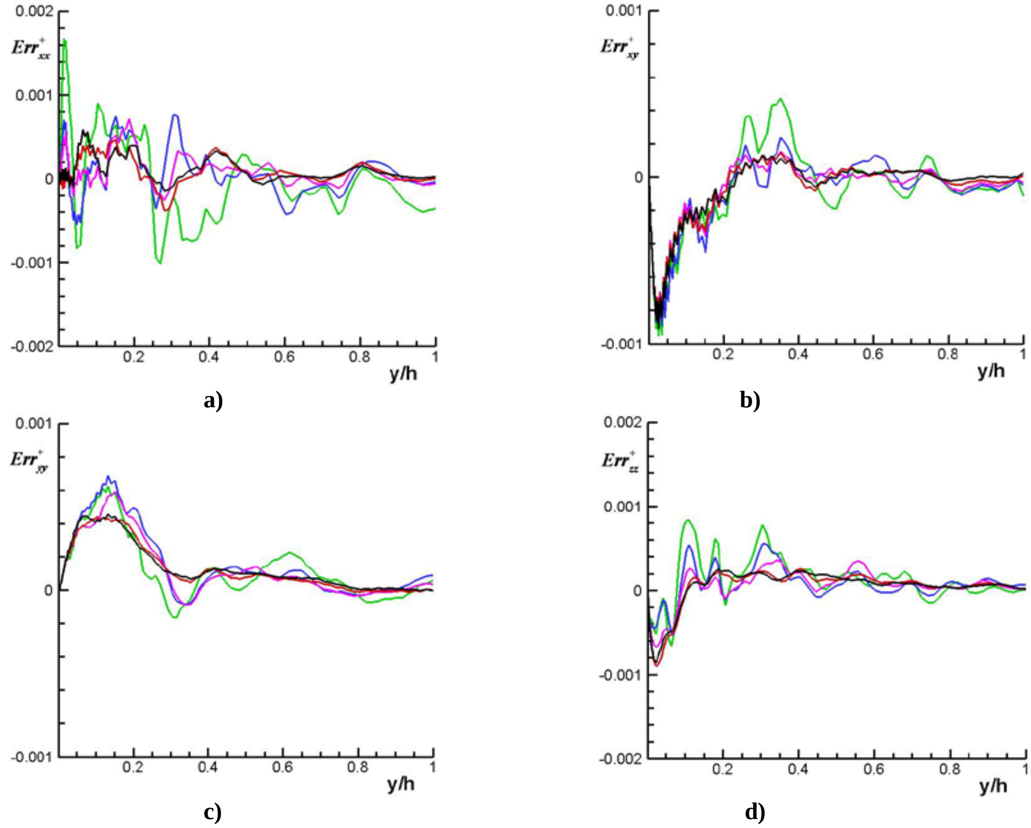

Figure 8. Balance errors in DNS budgets of the Reynolds stresses at different average times. Color scheme as in Fig. 3.

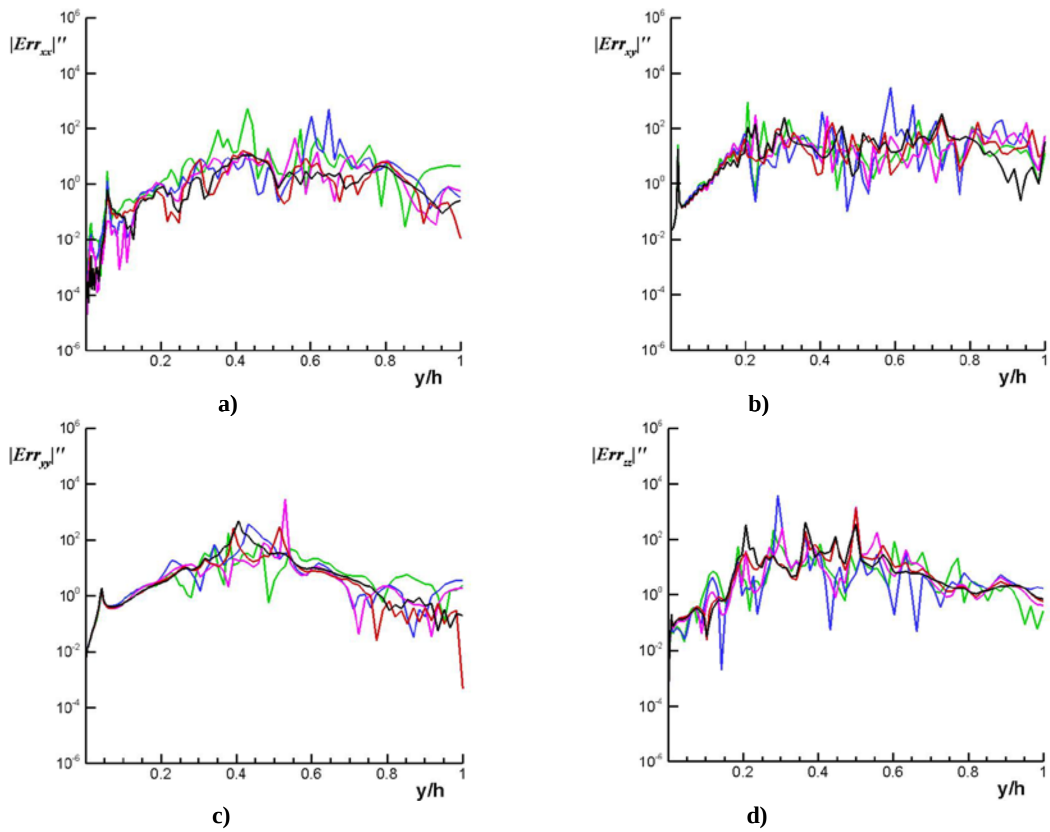

Figure 9. Ratios of balance errors to molecular diffusion in the DNS budgets of Reynolds stresses at different averaging times. Color scheme as in Fig. 3.

Acknowledgments

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