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A CRITERION FOR DETERMINING THE NEED FOR SCALE-RESOLVING SIMULATION AND DYNAMIC INTERFACE PLACEMENT IN HYBRID URANS-LES MODELING

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Abstract

Accurate prediction of turbulence production and dissipation remains a major challenge in turbulence modeling, particularly in near-wall regions where modeling assumptions often break down. In this work, the production terms in the transport equation for the dissipation rate are analyzed, and their corresponding closure models are assessed. The analysis reveals significant deficiencies in existing approaches. In particular, the commonly used closure for the production term in the transport equation of dissipation rate (ε) of two-equation RANS models, fails to capture the complex dynamics of the near-wall region, especially within the buffer layer. In addition, the eddy viscosity assumption is shown to be inadequate for representing Reynolds stresses, including the shear stress. These limitations can lead to poor representation of near-wall physics, even when larger-scale flow features are reasonably captured. Furthermore, a parameter is introduced as a practical indicator to assess the need for unsteady simulations beyond steady RANS and to identify regions requiring scale-resolving approaches. This parameter can be estimated from inexpensive preliminary simulations, providing a useful tool for guiding simulation strategy and grid refinement. Overall, the findings highlight the need for improved dissipation modeling, which is critical for enhancing the predictive capability of RANS models for large-scale systems and for improving the performance of hybrid URANS–LES turbulence modeling approaches.

Overview

Reynolds-Averaged Navier–Stokes (RANS) models are commonly employed to simulate high-Reynolds-number turbulent flows relevant to industrial applications. However, RANS methods are inherently limited in their ability to capture the essential unsteady dynamics of complex flows. Unsteady simulation techniques, such as wall-modeled large eddy simulation (WMLES) and hybrid URANS–LES approaches, offer promising intermediate strategies. However, these methods introduce their own modeling challenges (Bose and Park, 2018).

In this work, we propose a physics-based criterion derived from the dissipation-rate (ε) transport equation to determine whether scale-resolving simulation is warranted and to identify appropriate interface locations in hybrid URANS–LES frameworks. The proposed parameter is formulated in terms of the relative contributions of production mechanisms in the ε equation and can be estimated using RANS solutions, enabling an a priori assessment prior to performing computationally expensive unsteady simulations. More specifically, we analyze the sensitized RANS hybrid approach, e.g. the Scale adaptive Simulation (SAS) and its different formulations that use models based on Rotta's equation for integral length scale to transition from URANS dynamics to a scale-resolving mode through the energy dominant integral scales like that predicted by LES. It has been demonstrated that different formulations of SAS can successfully trigger the transition to scale-resolving mode and deliver results at an acceptable level of accuracy in massively separated flows (Mehdizadeh et al. 2014 and Menter and Egorov, 2010) and often fail to trigger such transition in attached and mildly separated flows where the base flow instability is insufficient. This issue was addressed in our previous investigation (Saini et al. 2023), and the improved triggering mechanism that considers deviations from equilibrium through a vortex stretching term in the turbulent dissipation rate and was shown to be responsive to non-equilibrium effects associated with the transition between URANS to Scale-resolving mode in attached flows. Additionally, it was shown that an appropriate length scale obtained through a transport equation for integral length scale for the gray area was necessary to allow an appropriate transition from URANS to scale-resolving mode to mitigate the Log-Layer Mismatch (LLM).

One of the remaining challenges in both WMLES and hybrid URANS-LES (in attached and mildly separated flows) is to (automatically and dynamically) locate/determine the appropriate interface location between URANS and LES in hybrid approach or off-wall location in WMLES (Bose and Park, 2018). In this work, we introduce a non-dimensional parameter based on flow characteristics that addresses this issue and provides an a-priori estimate of whether employing hybrid URANS–LES or WMLES would be appropriate. Specifically, this parameter could offer a means to assess whether unsteady simulations -other than DNS- are reasonable and justified [1].

[1]Communicated with K. Hanjalic

Dissipation rate equation and assessment of production term modeling

In an attempt to address this challenge, we revisit the exact transport equation for the dissipation rate (ε), which reads as follows (Hanjalic and Launder 2023):

$$\underbrace{\frac{D\varepsilon}{Dt} = -2\nu\left(\overline{\frac{\partial u_i}{\partial x_l}\frac{\partial u_k}{\partial x_l}} + \overline{\frac{\partial u_l}{\partial x_i}\frac{\partial u_l}{\partial x_k}}\right)\frac{\partial U_i}{\partial x_k}}_{P_{\varepsilon 1}+P_{\varepsilon 2}} \underbrace{-2\nu \overline{u_k \frac{\partial u_i}{\partial u_l}}\frac{\partial^2 U_i}{\partial x_l \partial x_k}}_{P_{\varepsilon 3}}$$
$$\underbrace{-2\nu\overline{\frac{\partial u_i}{\partial x_k}\frac{\partial u_i}{\partial x_l}\frac{\partial u_k}{\partial x_l}}}_{P_{\varepsilon 4}} \underbrace{-2\overline{\left(\nu\frac{\partial^2 u_i}{\partial x_k \partial x_l}\right)^2}}_{\Upsilon} + \underbrace{D_\varepsilon}_{Diffusion} \quad (1)$$

Note that in the equation above U_i and u_i and ν denote mean and fluctuating velocities and kinematic viscosity respectively.

$P_{\varepsilon 1,2,3,4}$, Υ and D_ε denote different production terms, destruction and diffusion respectively. Introduction of simple closure for $P_{\varepsilon 1}+P_{\varepsilon 2}$ and $P_{\varepsilon 4}-\Upsilon$ and further neglecting $P_{\varepsilon 3}$ results in the commonly used transport equation for ε in two-equation frameworks (please refer to (Hanjalić and Launder, 2023) for further details).

$$\frac{D\varepsilon}{Dt} = \underbrace{C_{\varepsilon 1}P_k\frac{\varepsilon}{k}}_{P_{\varepsilon 1}+P_{\varepsilon 2}} - \underbrace{C_{\varepsilon 2}\frac{\varepsilon^2}{k}}_{P_{\varepsilon 4}-\Upsilon} + D_\varepsilon, \quad (2)$$

where $C_{\varepsilon 1,2}$, k and $P_k = -\overline{u_i u_j}\frac{\partial U_i}{\partial x_j}$ are model constants, turbulent kinetic energy and its production respectively.

It should be noted that the model for $P_{\varepsilon 1}+P_{\varepsilon 2}$ was primarily developed based on dimensional arguments and has not been thoroughly evaluated, largely due to the lack of high-fidelity (DNS) data for these production terms. In this work, we assess the model using available DNS data for channel flow at two Reynolds numbers, $Re_\tau = 180, 1000$. Specifically, the model is evaluated by supplying it with DNS-based inputs for the shear stress, mean velocity, turbulent kinetic energy, and dissipation rate. The results indicate that the primary weakness of the model ($C_{\varepsilon 1}P_k\frac{\varepsilon}{k}$) in representing the combined production terms $P_{\varepsilon 1}+P_{\varepsilon 2}$ lies within the buffer layer, while predictions in the remainder of the channel are in reasonably good agreement with DNS data. However, the model fails to accurately capture the individual production terms, particularly in the near-wall region. (Figure 1)

To further investigate this behavior, the impact of employing an eddy-viscosity approach to model the shear stress is examined, while retaining DNS data as inputs (see Figure 2). The results show that the eddy-viscosity approach significantly overpredicts the production term, even when high-fidelity DNS data are provided. This clearly demonstrates that the eddy-viscosity assumption, particularly with a constant C_μ, is insufficient for accurately predicting the shear stress.

Finally, the performance of the eddy-viscosity approach is evaluated within full RANS simulations, where all inputs are obtained from RANS. Figures 1 and 2 summarize this comprehensive assessment. Although the use of RANS inputs appears to yield some improvement, this is likely coincidental and attributable to the reduced eddy viscosity in the near-wall region (see Figure 3). This behavior may also be specific to channel flow and not generally applicable to more complex configurations.

Additional source terms that include a second derivative of (mean) velocity mimicking $P_{\varepsilon 3}$ used in the SAS frameworks (Menter and Egorov, 2010 and by Mehdizadeh et al., 2014) successfully leverage the mean flow deformation available in strongly separated flows to trigger a transition from URANS to LES mode in such flows, and provide more accurate predictions compared to their underlying RANS models.

Regarding $P_{\varepsilon 4}$, it was shown in (Saini et al. 2023) that inclusion of a separate model for $P_{\varepsilon 4}$ in the ε equation provides greater sensitivity to triggering phenomena in addition to mean flow deformation, such as vortex filament (self)stretching resulting in successful triggering the transition from URANS to scale-resolving mode in attached/mildly separated flows. The following model was used for $P_{\varepsilon 4}$:

$$P_{\varepsilon 4} = C_{\varepsilon 4}\sqrt{Re_t}\frac{\varepsilon^2}{k} \quad (3)$$

with Re_t being the turbulent Reynolds number and $C_{\varepsilon 4} = 0.25$, see (Saini et al., 2023) for further details. Figure 4 compares model predictions obtained using inputs from DNS data and from RANS simulations with the corresponding DNS results. Results suggest that except for near-wall region, the model is capable of capturing the behavior of $P_{\varepsilon 4}$.

Development of a criterion for assessing the need for scale-resolving simulation

A closer look into the ε equation reveals that if the Reynolds number (local Reynolds number) is high enough such that the Kolmogorov theory (K41) holds true, i.e., turbulence is in equilibrium and the dissipation only happens at Kolmogorov scales that are isotropic, all production terms and in particular $P_{\varepsilon 1,2}$ become negligible. In fact this could be mathematically shown that if small dissipating eddies are isotropic, these production terms are zero in incompressible flows. We will leverage this and assess the ratio of $\frac{P_{\varepsilon 4}}{P_{\varepsilon 1}+P_{\varepsilon 2}}$, denoted as R_p, in turbulent channel flow to determine if this ratio can help identify regions where conducting LES would be reasonable. It should be noted that $P_{\varepsilon 3}$ generally has a very negligible effect except for strongly separated flows where mean flow deformation occurs.

Figure 5(a) demonstrates the only available DNS results for $R_p = \frac{P_{\varepsilon 4}}{P_{\varepsilon 1}+P_{\varepsilon 2}}$ and compares them to the results of models for $P_{\varepsilon 1}+P_{\varepsilon 2}$ and $P_{\varepsilon 4}$, obtained using DNS data as input. It can be concluded that the models for the production terms are reasonably accurate in predicting R_p, at least in terms of capturing the overall trend. We continue our analysis and evaluate R_p for additional Reynolds number up to $Re_\tau = 8000$ shown in figure 5(b). Next, we identify the location (y^+) at which the contribution of $P_{\varepsilon 1}+P_{\varepsilon 2}$ becomes negligible, i.e. $P_{\varepsilon 4}$ becomes at least one order of magnitude larger than $P_{\varepsilon 1}+P_{\varepsilon 2}$ ($R_p \approx O(10)$). For the lowest Reynolds number, i.e.,$Re_\tau = 180$, this ratio approaches 10 around the channel center line ($y^+ \simeq 160$), which means virtually no region exists where performing LES would be reasonable. As the

Reynolds number increases, the region in which conducting LES is reasonable progressively expands. This analysis may suggest R_p might serve as a criterion to identify regions where performing unsteady simulations such as LES and hybrid URANS/LES are justifiable [2].

Next, we evaluate this ratio within a RANS simulation. In particular, we conducted several RANS simulations using a modified version of the $k-\zeta-\varepsilon-f$ model (Laurence et al., 2005) that was used as underlying RANS model in our hybrid framework (Saini et al. 2023). Consistent with the previous findings using DNS data as input to the models for the production terms, the RANS based assessments demonstrate that for the lowest Reynolds numbers ($Re_\tau 180 and 1000$), there is virtually not enough space to initiate a transition to scale-resolving mode and thus only DNS would be the most appropriate unsteady simulation method. For higher Reynolds numbers our assessments confirm conducting unsteady simulation was reasonable, however, the locations at which R_p approaches $O(10)$ were different than those using DNS data as input. Nonetheless, they were consistent with previous finding.

Results and Discussion

The proposed criterion was subsequently implemented within the proposed hybrid framework (Saini et al. 2023) to assess its capability to dynamically determine the interface location. Three different mesh resolutions(detailed in table 1) have been used to assess the sensitivity of the criterion to mesh resolution as well. Figure 6a presents the instantaneous interface position obtained on-the-fly for channel flow at $Re_\tau = 8000$ using different grid resolutions. The results demonstrate that the criterion provides a physically consistent interface location while exhibiting limited sensitivity to grid resolution. This feature is particularly advantageous, as most hybrid approaches have been reported to display inconsistent responses to grid refinement (Saini et al., 2018).

It should also be noted that when the grid resolution becomes significantly finer than the integral length scale in the transition region (the "Grey Area"), large developing eddies may be artificially over-resolved (i.e., fragmented). We suspect that such over-resolving potentially leads to some deviations from DNS in the mean velocity profile observed in figure 6b. The results presented in this manuscript are therefore preliminary and are intended to assess the capability of the proposed criterion; more comprehensive studies, including channel flows at different Reynolds numbers and more complex geometries, are currently underway.

Summary and potential future direction

In summary, the proposed parameter R_p may serve as a practical criterion for assessing whether unsteady simulations, beyond DNS, are warranted and, if so, for identifying the regions where they should be applied. More importantly, R_p can be estimated from relatively inexpensive (potentially two-dimensional) RANS simulations prior to undertaking computationally intensive unsteady calculations. This capability can also guide the design of more appropriate computational grids and help avoid unnecessary refinement. However, the results demonstrate that the existing models for various production terms, particularly the model for $P_{\varepsilon 1}+P_{\varepsilon 2}$, exhibits significant deficiencies in capturing near-wall dynamics, especially within the buffer layer. In addition, the eddy-viscosity-based modeling of Reynolds stresses, including shear stress, has been shown to be inaccurate.

Overall, given the importance of the dissipation rate in hybrid URANS–LES modeling, and the potential of RANS approaches to simulate large-scale, high-Reynolds-number flows, addressing these shortcomings is essential. In this context, improving dissipation-rate modeling using emerging approaches, such as machine-learning-based methods, appears to be a promising direction.

[2] Communicated with K. Hanjalic

TABLES

Table 1: Flow domain and mesh resolution details, with h being channel half height, and $N_{x,y,z}$ number of grids in the streamwise, wall normal and spanwise directions.

Flow domain	$2\pi \times 2h \times \pi$		
Re_τ	8000		
Mesh Resolution	N_x	N_y	N_z
fine mesh	96	128	96
medium mesh	80	104	80
ultra fine mesh	128	192	128

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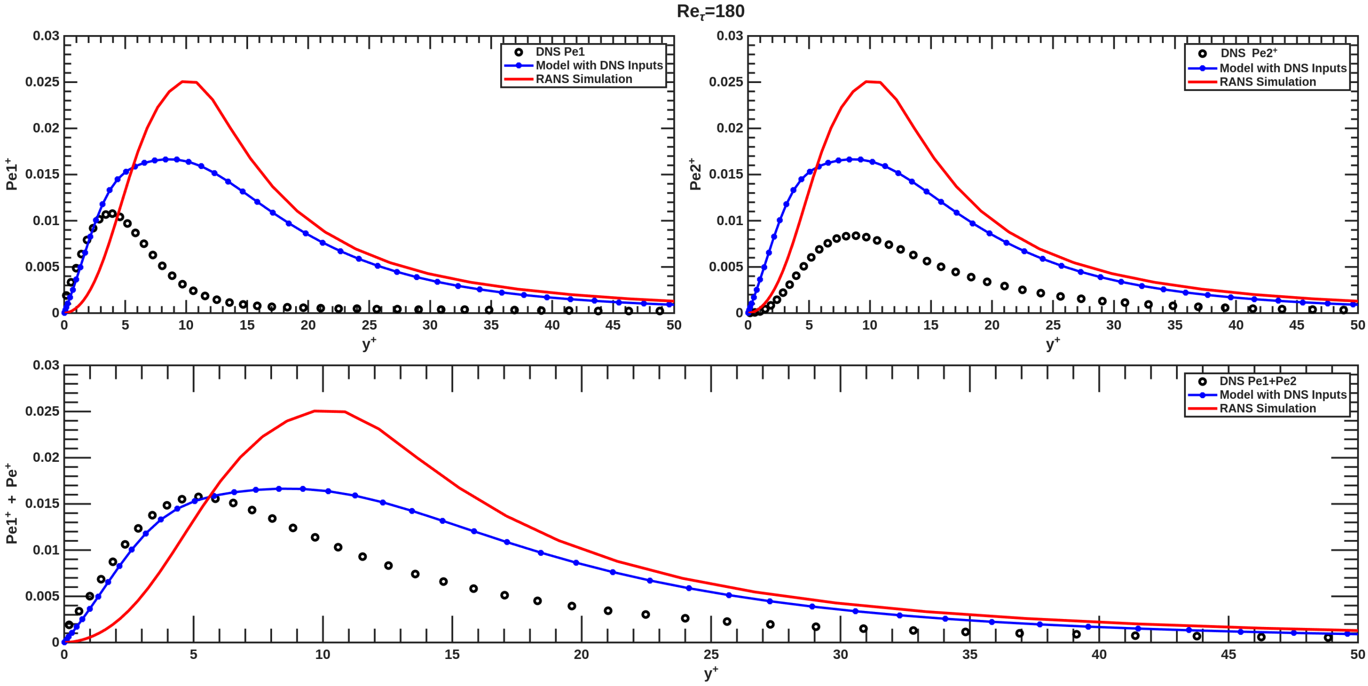

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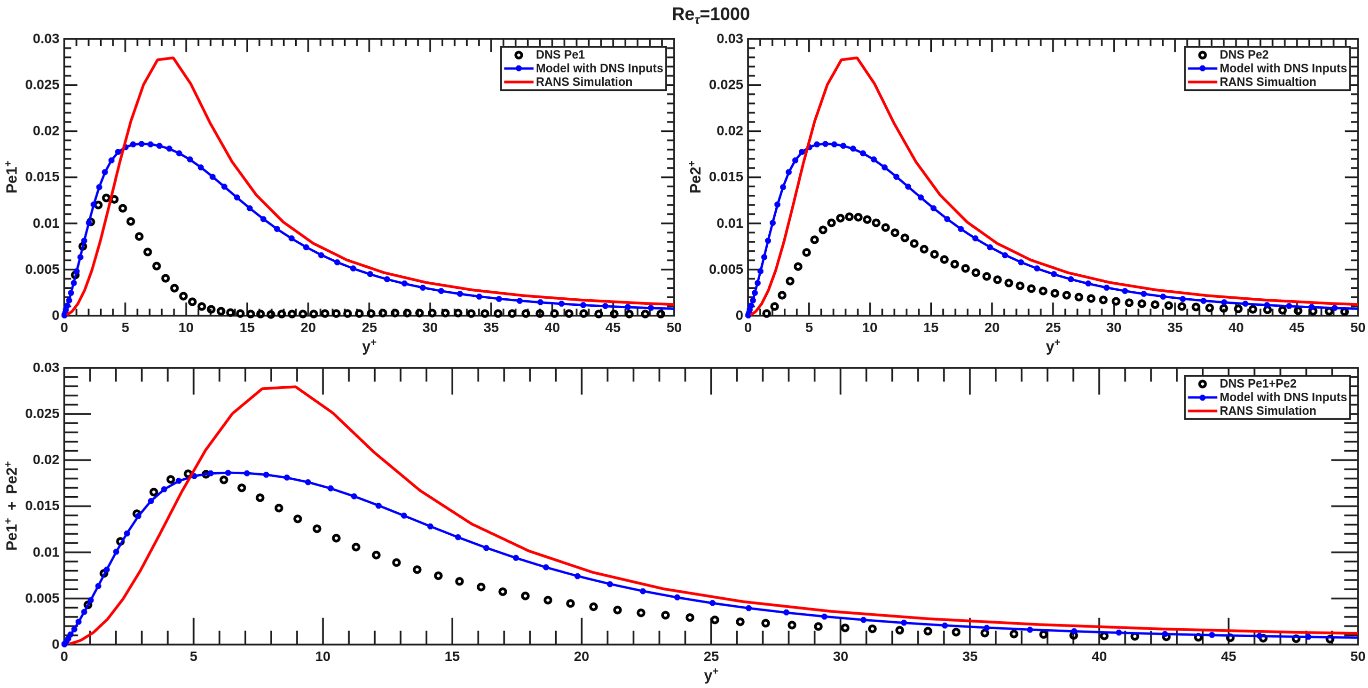
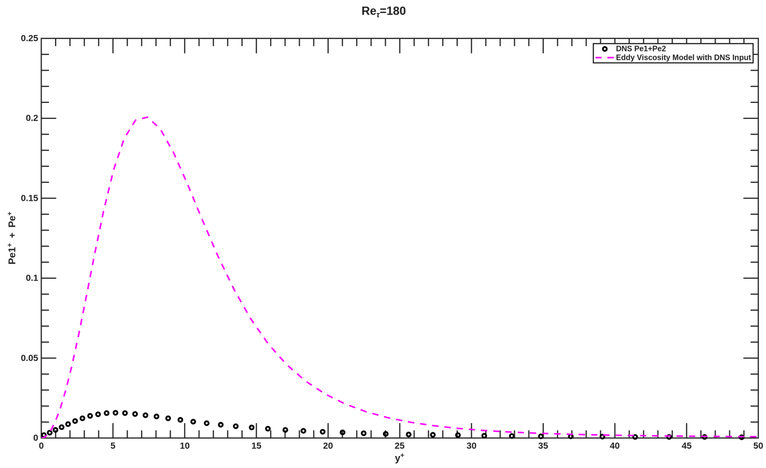


(b)

Figure 1: Assessment the validity of the model (i.e., $C_{\varepsilon 1} P_k \frac{\varepsilon}{k}$), for $P_{\varepsilon 1} + P_{\varepsilon 2}$ in the ε transport equation at two Reynolds numbers $Re_\tau = 180$ (a); $Re_\tau = 1000$, (b); Blue: DNS data as input for $C_{\varepsilon 1} P_k \frac{\varepsilon}{k}$; Red: RANS simulation with eddy viscosity model; ○: DNS



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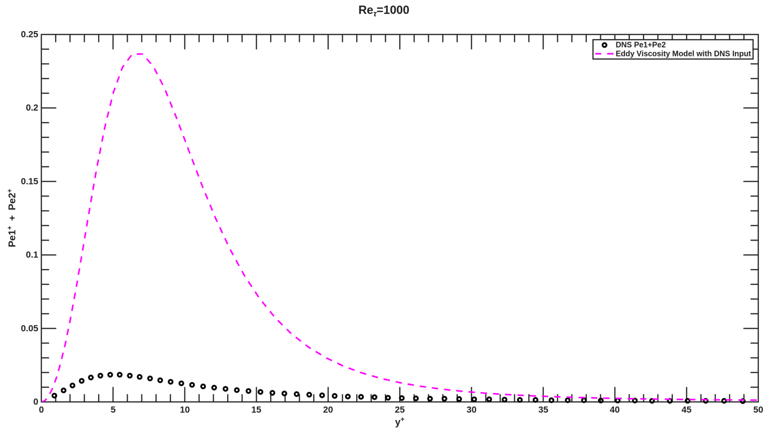
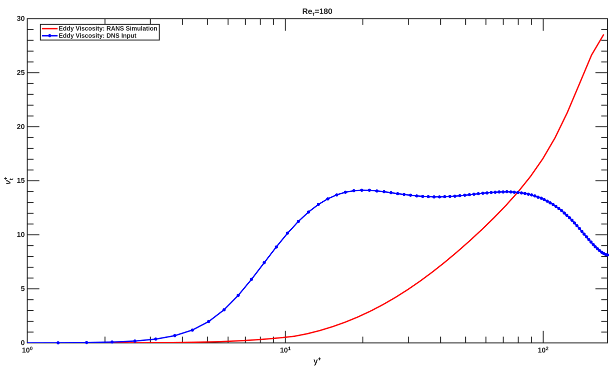


(b)

Figure 2: Assessment of predictive capability of $C_{\varepsilon 1} P_k \frac{\varepsilon}{k}$ model for $P_{\varepsilon 1} + P_{\varepsilon 2}$, using eddy viscosity approach to model the shear stress with DNS data as input, at two Reynolds numbers $Re_\tau = 180$ (a); $Re_\tau = 1000$, (b)



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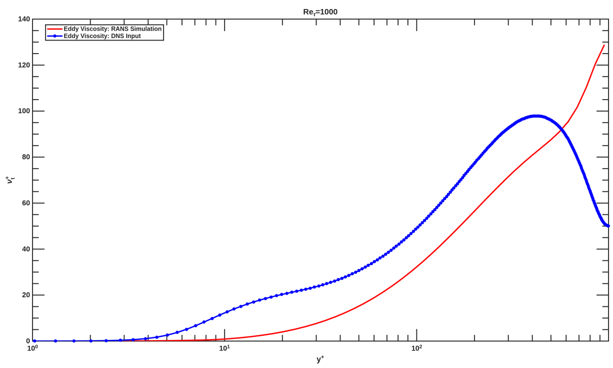
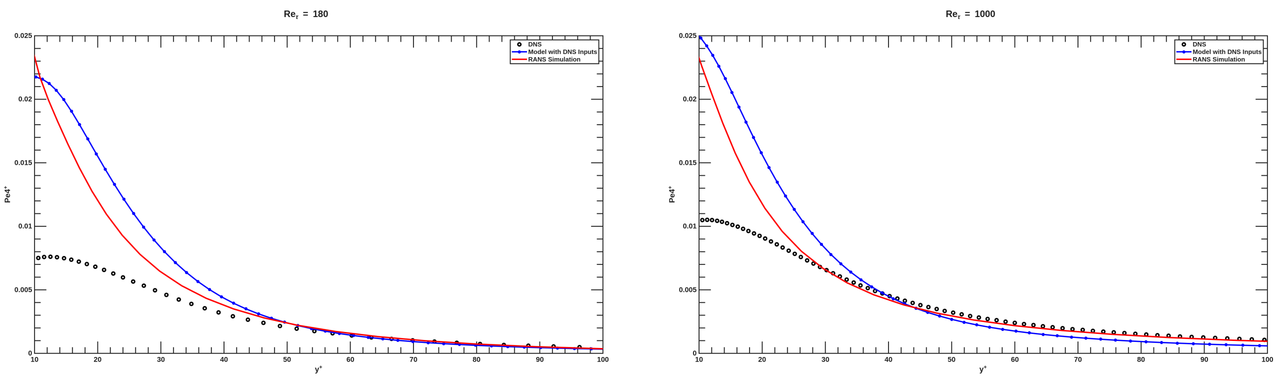


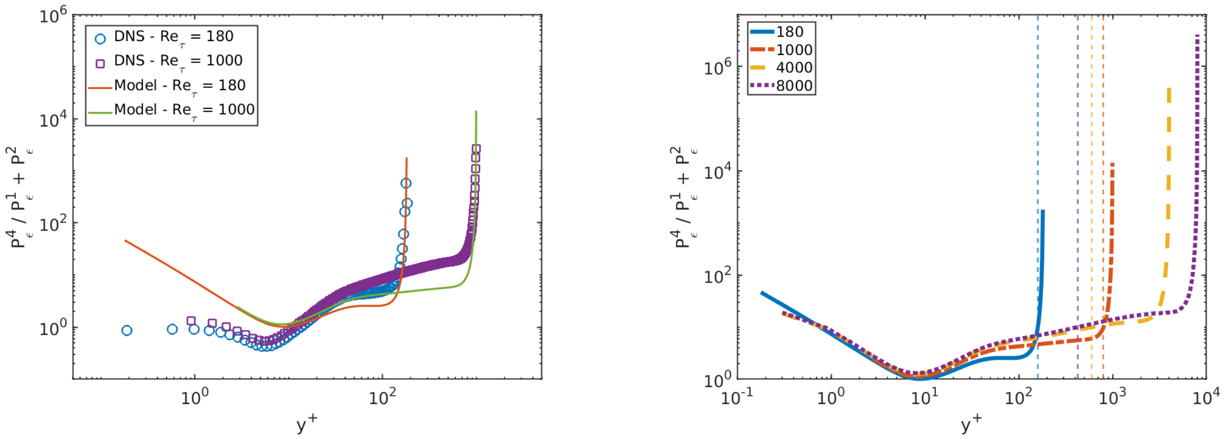
(b)

Figure 3: Dimensionless eddy viscosity $C_\mu \frac{k^2}{\varepsilon}$; Blue: calculated using DNS data as input; Red: obtained from RANS simulation; (a) $Re_\tau = 180$, (b) $Re_\tau = 1000$



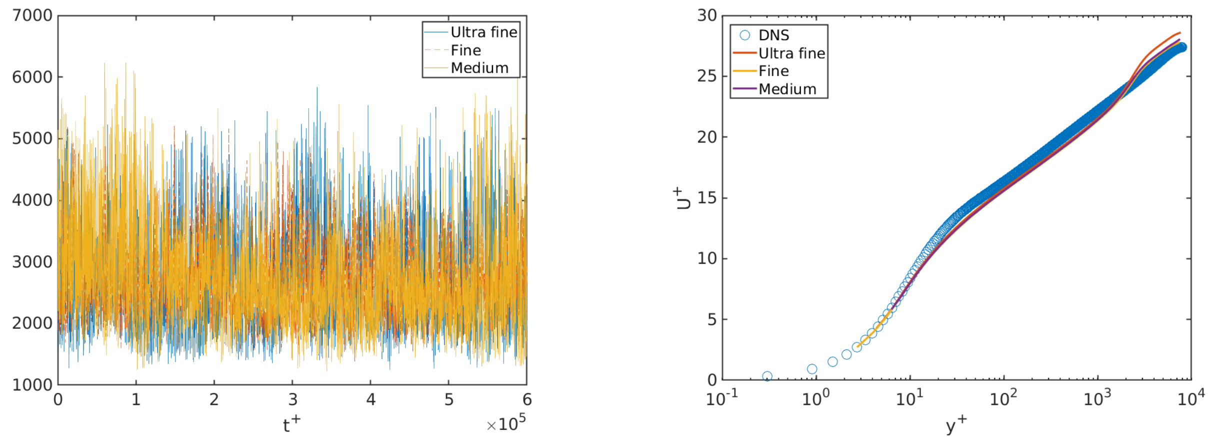
(a) (b)

Figure 4: (Assessment the validity of the model for $P_{\varepsilon 4}$ (i.e., $C_{\varepsilon 4}\sqrt{Re_t}\frac{\varepsilon^2}{k}$), for $P_{\varepsilon 4}$ in the ε transport equation at two Reynolds numbers, (a) $Re_\tau = 180$; (b) $Re_\tau = 1000$; Blue: DNS data as input for the model; Red: RANS simulation with eddy viscosity model; ○: DNS



(a) (b)

Figure 5: (a) Assessment the validity of production models in the ε equation forming R_p and, (b), evaluate R_p for channel flow at different Reynolds number, using DNS data as input for the production terms



(a) (b)

Figure 6: (a) Instantaneous interface location determined dynamically using R_p criterion with average value of y^+ around 2700 for all three resolutions and, (b), the streamwise mean velocity for turbulent channel flow at $Re_\tau = 8000$