A Unified RANS-LES Model. Part 1. Computational Model Development

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Abstract

Large eddy simulation (LES) is computationally extremely expensive for the investigation of wall-bounded turbulent flows at high Reynolds numbers. A way to reduce the computational cost of LES by orders of magnitude is to combine LES equations with Reynolds-averaged Navier-Stokes (RANS) equations used in the near-wall region. A huge variety of such hybrid RANS-LES methods are currently in use such that there is the question of which hybrid RANS-LES method represents the optimal approach. The properties of an optimal hybrid RANS-LES model are formulated here by taking reference to fundamental properties of fluid flow equations. It will be shown that unified RANS-LES models derived from an underlying stochastic turbulence model have the properties of optimal hybrid RANS-LES models. The question of how unified RANS-LES models can be computationally developed is addressed. *A-priori* analyses of channel flow data are used for a thorough analysis of different RANS-LES coupling methods. The application of a dynamic RANS-LES coupling approach is identified to represent the most convenient computational approach. *A-posteriori* analyses of channel flow data are used to demonstrate that the computational model obtained does also satisfy all the properties of an optimal hybrid RANS-LES model.

Keywords: Stochastic turbulence model, RANS, LES, Unified RANS-LES models, Channel flow application

1. Introduction

The use of direct numerical simulation (DNS) to numerically integrate the basic equations of fluid mechanics and thermodynamics is extremely helpful for studying the fundamental mechanisms of turbulent flows, but the computational cost of DNS do not allow investigations of complex engineering and environmental flows. For example, the number of grid points N required to perform DNS of turbulent channel flow scales with the Reynolds number Re according to $N \sim Re^{2.7}$ [1, 2]. A solution for this cost problem requires the use of modeling assumptions for at least a part of the spectrum of turbulent motions.

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There are two ways that have been used to address this issue. The first way, deterministic [2–9] or stochastic [10–17] large eddy simulation (LES) methods, applies modeling assumptions to small-scale turbulent motions while the energetic large scale structures are resolved. The second way, deterministic [2, 18, 19] or stochastic [2, 20–22], Reynolds-averaged Navier-Stokes (RANS) methods, applies modeling assumptions to all the scales of motion. The use of LES methods is much cheaper than DNS regarding the simulation of complex free shear flows: the total number of grid points required scales as $N \sim Re^{0.4}$ [23]. However, for wall-bounded flows the cost of fully resolved LES scales as $N \sim Re^{1.76}$ [24, 25], which is comparable to DNS. Therefore, it is very expensive to use LES for simulations of complex wall-bounded engineering and environmental flows at high Reynolds numbers. The use of RANS methods can reduce the computational cost of complex wall-bounded flow simulations. The number of grid points required to perform RANS simulations of wall-bounded flows is independent of the Reynolds number along the streamwise and spanwise directions and scales as $N \sim \ln Re$ along the wall normal direction [2]. However, there are two issues associated with the use of RANS models for turbulent flow simulations. First, the accuracy of numerical predictions depends on the choice of the RANS model ($k-\epsilon$, $k-\omega$, etc.) and flow considered (separated flows, swirling flows, etc.) [19]. Therefore, RANS predictions have to be validated by experimental or DNS data. Second, RANS models do not provide instantaneous flow fields, which have to be considered in many applications such as aircraft noise predictions, swirling flows, etc.

The prohibitive cost of LES, in particular for the investigation of wall-bounded flows at high Reynolds numbers, motivated the development of hybrid RANS-LES methods. In the hybrid RANS-LES modeling approach, a part of the flow domain (the near-wall region) is modeled using RANS methods and the remaining flow domain (away from the wall) is modeled using LES methods. The use of hybrid RANS-LES methods has three main advantages. First, hybrid RANS-LES methods can be used to simulate flows at high Reynolds numbers, which would not be feasible with pure LES [26]. Second, hybrid RANS-LES methods can provide instantaneous flow fields. Third, compared to pure RANS methods, the use of hybrid RANS-LES methods reduces the influence of the choice of the RANS model applied. These advantages make the use of hybrid RANS-LES methods highly attractive regarding the study of complex engineering and environmental flows at high Reynolds numbers. To illustrate the advantages of using hybrid RANS-LES methods for complex turbulent flow simulations, let us consider the turbulent flow past a sphere. This flow configuration is representative for most external engineering flows. The flow consists of an attached boundary layer, developed upstream of the sphere, and flow separation in the downstream wake region. At low and moderate Reynolds numbers, this flow can be investigated using DNS and LES methods, respectively. However, at high Reynolds numbers either RANS or hybrid RANS-LES methods are required for the numerical simulation. The use of RANS methods has been shown to be inaccurate even for the prediction of the Strouhal number of such flows [27]. However, the use of hybrid methods (RANS in the attached boundary layer and LES in the wake region) led to successful predictions of the Strouhal number and aerodynamic forces on the surface of the sphere, and it provided unsteady flow fields in the downstream wake [28].

Despite their success, there are several problems related to existing hybrid RANS-LES methods. First, there is a huge variety of hybrid RANS-LES methods, and most of these methods have been empirically developed (only a few researchers developed hybrid RANS-LES methods on a theoretical basis [21, 29–34]). Hence, it is needed to clarify the most appropriate theoretical basis for developing hybrid RANS-LES methods. Second, most existing hybrid RANS-LES methods do not represent hierarchical (stress transport equation, nonlinear and linear algebraic stress) models, which can be used to address problems of varying complexity. Third, the predictions of most existing hybrid RANS-LES methods have shortcomings, e.g., regarding the mean velocity profile in the log-law region of attached boundary layers [35–38] and the anisotropy of Reynolds stresses in near-wall regions.

The purpose of this paper is to develop computationally the realizable unified RANS-LES models derived by Heinz [33] on the basis of stochastic analysis, and to evaluate the characteristic features of these models. This will be done in terms of *a-priori* and *a-posteriori* analyses of turbulent channel flow data. The paper is organized in the following way. An overview of existing hybrid RANS-LES methods is given in Sect. 2. Sect. 3 describes the properties of an optimal hybrid RANS-LES model and shows that the unified models derived by Heinz [33] on the basis of stochastic analysis satisfy the properties of an optimal model. Sects. 4, 5, and 6 describe coupling options of RANS and LES equations, the unified model applied in the following and the computational approach. Analyses of the performance of various computational RANS-LES coupling approaches and basic properties of the implied hybrid RANS-LES methods are presented in Sects. 7 and 8. The conclusions are summarized in Sect. 9.

2. Existing Hybrid RANS-LES Methods

Let us begin with the consideration of LES and RANS methods. Depending on the model formulation as RANS or LES model, $\widetilde{U}_i$ refers to the mean or filtered velocity. For simplicity, we consider incompressible flow, i.e., $\widetilde{U}_i$ satisfies $\partial \widetilde{U}_k / \partial x_k = 0$. The conservation equation of momentum is given by

$$\frac{\widetilde{D}\widetilde{U}_i}{\widetilde{D}t} + \frac{\partial D_{ik}}{\partial x_k} = -\frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_i} + 2\nu \frac{\partial \widetilde{S}_{ik}}{\partial x_k}. \tag{1}$$

Here, $\widetilde{D}/\widetilde{D}t = \partial/\partial t + \widetilde{U}_k \partial/\partial x_k$ denotes the filtered Lagrangian time derivative, and $\widetilde{S}_{ij} = (\partial \widetilde{U}_i/\partial x_j + \partial \widetilde{U}_j / \partial x_i)/2$ is the rate-of-strain tensor. In addition, we have here the pressure $\langle p \rangle$, ρ is the constant mean mass density, and ν is the constant kinematic viscosity. The sum convention is used throughout this paper. Equation (1) is unclosed due to the unknown stress tensor D_{ij}. This stress is usually parametrized as $D_{ij} = kF_{ij}[\widetilde{\boldsymbol{S}}\ L_0/k^{1/2},\ \widetilde{\boldsymbol{\Omega}}\ L_0/k^{1/2}]$. Here, $k = D_{nn}/2$ refers to the turbulent kinetic energy, and F_{ij} is a non-dimensional functional involving in addition to $k^{1/2}$ the rate-of-strain matrix $\widetilde{\boldsymbol{S}}$ with elements $\widetilde{S}_{ij}$, the rate-of-rotation matrix $\widetilde{\boldsymbol{\Omega}}$ with elements $\widetilde{\Omega}_{ij} = (\partial \widetilde{U}_i/\partial x_j - \partial \widetilde{U}_j/\partial x_i)/2$, and a characteristic length scale L_0. Depending on the definition of L_0, Eq. (1) can be used either as a RANS or LES equation. An LES equation is given if L_0 is defined to be proportional to the filter width Δ, which represents an external parameter that has to be provided. A RANS equation is given if L_0 is provided as a characteristic length scale of large-scale turbulence. A difference is often made between RANS and unsteady RANS

(URANS) methods, with the understanding that RANS methods provide time-independent solutions, whereas URANS methods provide time-dependent solutions [27]. For simplicity, we will not distinguish between such different types of solutions and only talk about RANS methods. Corresponding to the terminology used for RANS methods, no difference will be made between LES and Very Large Eddy (VLES) methods.

It turns out that there are many different possibilities to combine RANS and LES methods. Coupled RANS-LES methods are the most commonly used methods. There are two basic ways to couple RANS and LES methods: segregated RANS-LES methods, which use different velocity equations and couple all mean flow and turbulence variables at an interface, and interfaced RANS-LES methods, which use one velocity equation and couple the stress D_{ij} at an interface. The use of segregated methods is described in a variety of applications [27, 39–49]. A general problem is the coupling of RANS and LES variables at the interface. In general, experimental data (which are often unavailable) are required to demonstrate the suitability of RANS results, and an empirical noise model is needed to create instantaneous LES inflow data on the basis of RANS results [47, 50]. Compared to segregated methods, the significant advantage of interfaced methods is the continuous velocity transition between RANS and LES subdomains without discontinuity at the interface [35–38, 51–58]. The most commonly used interfaced approach is the detached eddy simulation (DES) of Spalart et al. [51]. The DES model has been successfully applied to many massively separated flow configurations [35, 51–53]. However, the discontinuous calculation of RANS and LES stresses at the interface implies a jump in the mean velocity profile in the log-law region near the RANS-LES interface (i.e., a spurious buffer layer) of attached flows. Different empirical methods [35, 56, 57] have been proposed to avoid the occurrence of this spurious buffer layer. These empirical methods successfully reduced the size of the spurious buffer layer for the flows investigated, but the applicability of these emprirical approaches to a wide range of flows still has to be investigated. Similar problems regarding the use of other interfaced methods for simulations of attached boundary layers were reported by Breuer et al. [36], Davidson and Peng [37], Hamba [38], Tucker and Davidson [54], Tessicini et al. [55], Kniesner et al. [58].

Another way of combining RANS and LES methods is the use of distributed RANS-LES methods. There are two basic ways of designing such methods: mixed (or blended) RANS-LES methods, which use one velocity equation in conjunction with a combination of RANS and LES stresses at every point, and non-mixed methods, which use one velocity equation in conjunction with either a RANS or LES stress at every point depending on a local criterion that varies smoothly in space. Distributed methods, which have the advantages of being independent of the problems introduced by interfaces, were developed in a variety of alternative ways. Mixed RANS-LES methods were presented, for example, by Speziale [59], Germano [29], and Girimaji [32]. Applications of Speziale's flow simulation methodology can be found in [60–62], applications of Germano's hybrid filtering approach can be found in Sánchez-Rocha and Menon [34], Sagaut and Germano [63], Rajamani and Kim [64], Fadai-Ghotbi et al. [65], Sánchez-Rocha and Menon [66], and applications of Girimaji's Partially Averaged Navier-Stokes Equations (PANS) approach can be found in [67–74] . Non-mixed RANS-LES methods were developed by Heinz on the basis of the mean velocity equation [21] and on the more general basis of stochastic turbulence models [33]. Only preliminary applications of Heinz's model were reported so far [75, 76]. Merci et al. [30] used a corresponding formulation of the velocity equation in conjunction with the application of renormalization group theory for the calculation of the subgrid-scale (SGS) viscosity. Applications of Merci's approach were reported by De Langhe et al. [31, 77, 78].

3. A Unified RANS-LES Model

The discussion in the preceding section shows that there is a variety of possibilities to design hybrid RANS-LES methods. Apart from that, many of these methods can be used in several ways, e.g., depending on how the stresses $D_{ij} = kF_{ij}[\widetilde{\boldsymbol{S}}\, L_0/k^{1/2},\ \widetilde{\boldsymbol{\Omega}}\, L_0/k^{1/2}]$ are combined. For example, it is possible to transition from LES to RANS by matching the RANS and LES stresses D_{ij}, or the coefficients $L_0 k^{1/2}$ (turbulent viscosities) of $\widetilde{\boldsymbol{S}}$ and $\widetilde{\boldsymbol{\Omega}}$, or the length scales L_0, or the time scales $L_0/k^{1/2}$. So how is it possible to determine the most appropriate hybrid RANS-LES method?

A basis for addressing this question is given by the general properties of fluid flow equations. The simplest way to see these properties is to consider molecular motion equations [33, 79] that imply the Navier-Stokes equations (see, e.g., equation (2.9b) in reference [33]). These equations are characterized by the following: they represent a realizable fluid flow model that is supported by a proven theory, and the fluid model involves two ingredients: (a) a model for the evolution of velocities in a nondimensional time defined in terms of a characteristic time scale, and (b) a model for the characteristic time scale used to define the nondimensional time. An optimal hybrid RANS-LES model should reflect these fundamental properties of fluid flow equations and have the following properties P1, P2, and P3:

P1: The hybrid RANS-LES model is supported by a proven theory and realizable.

P2: Scale information enters the hybrid model only via the time scale model.

P3: The model for the time scale describes continuous variations between the RANS and LES scale.

Property P1 is relevant to the understanding of the range of applicability of simulation methods. Realizability was proven to represent a valuable guiding principle for turbulence modeling [2, 80–83]. Therefore, an optimal hybrid RANS-LES model should satisfy the property P1. An optimal hybrid RANS-LES model should reflect the relevant property of RANS and LES equations to involve the same velocity model, i.e., the hybrid model should satisfy the property P2. In this way, an optimal hybrid model minimizes the use of modeling assumptions, which are focused on the explanation of time scale variations. The design of a hybrid RANS-LES model then requires that the transition between RANS and LES equations is controlled by a model for the characteristic time scale. An optimal hybrid model will involve a time scale model that describes continuous variations between the RANS and LES scale, which corresponds to property P3. A model that has this property enables simulations without discontinuities or jumps of mean velocity profiles near interfaces. A combination of velocity and time scale models that have the properties P2 and P3 represents a unified turbulence model because it combines on velocity model with a unified time scale formulation that covers both the RANS and LES scale.

Most hybrid RANS-LES methods described in Sect. 2 do not satisfy all the properties P1, P2, and P3. For example, many hybrid methods are based on *ad hoc* assumptions, which means there is no underlying theory that can explain the structure of equations applied. It is then unclear, for example, in which way such models can be extended to nonlinear stress models. Many methods do also not satisfy the properties P2 and P3 because scale variations are not only covered by variations of one scale-determining time scale, which corresponds to the use of different velocity models in RANS and LES limits. The purpose here is not to provide an analysis of properties of all available hybrid RANS-LES models. Instead, the goal is to show that the unified models derived by Heinz [33] on the basis of stochastic analysis satisfies the properties P1, P2, and P3, and to further investgate the suitability of these models.

Heinz's unified model [33] was developed as a model for the evolution of the probability density function (PDF) of turbulent velocities. Incompressible flow is considered again (the compressible formulation can be found elsewhere [33]). The unified model enables the derivation of transport equations for all the moments of the PDF. The model does exactly reproduce the incompressibility constraint $\partial \widetilde{U}_k/\partial x_k = 0$ and the conservation of momentum equation (1). For the stress tensor, which appears as an unknown in the momentum equation, the PDF model implies the equation

$$\frac{\widetilde{D} D_{ij}}{\widetilde{D}t} + \frac{\partial T_{kij}}{\partial x_k} = -D_{ik}\frac{\partial \widetilde{U}_j}{\partial x_k} - D_{jk}\frac{\partial \widetilde{U}_i}{\partial x_k} - \frac{2}{\tau_L}\left(D_{ij} - \frac{c_o}{3}D_{kk}\delta_{ij}\right). \tag{2}$$

Here, T_{ijk} is the triple correlation tensor of velocity fluctuations, τ_L is the Lagrangian relaxation time scale of turbulent velocity fluctuations, and c_o is a model constant. For the following discussion it is helpful to rewrite Eq. (2) for D_{ij} in terms of equations for the turbulent kinetic energy $k = D_{nn}/2$ and standardized anisotropy tensor $d_{ij} = (D_{ij} - 2k\delta_{ij}/3)/(2k)$. These equations are given by [33]

$$\frac{\widetilde{D}k}{\widetilde{D}t} + \frac{1}{2}\frac{\partial T_{knn}}{\partial x_k} + 2kd_{kn}\frac{\partial \widetilde{U}_n}{\partial x_k} = -\frac{2(1-c_o)k}{\tau_L}, \tag{3}$$

$$\frac{\widetilde{D}d_{ij}}{\widetilde{D}t} + \frac{1}{2k}\frac{\partial (T_{kij} - T_{knn}\delta_{ij}/3)}{\partial x_k} + \frac{d_{ij}}{k}\frac{\widetilde{D}k}{\widetilde{D}t} + d_{ik}\frac{\partial \widetilde{U}_i}{\partial x_k} - \frac{2}{3}d_{kn}\frac{\partial \widetilde{U}_n}{\partial x_k}\delta_{ij} = -\frac{2}{\tau_L}d_{ij} - \frac{2}{3}\widetilde{S}_{ij}. \tag{4}$$

These equations can be used to derive a consistent hierarchy of deterministic models, which is helpful for working with models that are chosen according to the complexity of the flow considered. One option of using Eqs. (1), (3), and (4) is to close these equations by a model for the triple correlation T_{ijk}, which is implied by the PDF transport equation considered [21, 84]. A second option is to reduce the computational effort significantly by using Eq. (4) for the development of an algebraic model for the stress D_{ij}. A first-order approximation for D_{ij} can be obtained by neglecting the left-hand side terms in Eq. (4), which results in $d_{ij}^{(1)} = -\widetilde{S}_{ij}\tau_L/3$. The latter expression implies that D_{ij} is found in the first order of approximation as

$$D_{ij}^{(1)} = \frac{2}{3}k\delta_{ij} - 2\nu_t\widetilde{S}_{ij}, \tag{5}$$

where the turbulent viscosity ν_t is given by $\nu_t = k\tau_L/3$. A better model for D_{ij} is given by the following second-order approximation [33]

$$D_{ij}^{(2)} = D_{ij}^{(1)} + \frac{3\nu_t^2}{k}\left[2\widetilde{S}_{ik}\widetilde{S}_{kj}^d - \frac{2}{3}\widetilde{S}_{nk}^d\widetilde{S}_{kn}\delta_{ij} - \widetilde{S}_{ik}\widetilde{\Omega}_{kj} - \widetilde{S}_{jk}\widetilde{\Omega}_{ki}\right]. \tag{6}$$

The latter expression can be obtained by neglecting the transport terms (the first three terms) and using the first-order approximation $d_{ij}^{(1)} = -\widetilde{S}_{ij}\tau_L/3$ to replace d_{ij} in the production terms on the left-hand side of Eq. (4).

These linear and quadratic unified models satisfy the properties P1, P2, and P3 of an optimal hybrid RANS-LES model. The unified models presented here satisfy the property P1. These stress models are implied by the underlying stochastic turbulence model, which is well supported [33]. Realizability is guaranteed in the sense that these equations are derived as a consequence of a realizable stochastic turbulence model. A further discussion of the realizability problem is given in Sect. 8.1. Property P2 is also satisfied: RANS and LES equations have the same structure. The only difference is given by the specification of the time scale τ_L applied. Property P3 can be satisfied by defining the time scale in the following way Heinz [33],

$$\tau_L = min(\tau_L^{LES}, \tau_L^{RANS}). \tag{7}$$

Here, τ_L^{LES} and τ_L^{RANS} represent typical time scales used in LES and RANS approaches. According to this definition, Eq. (1) combined with Eq. (2) (or Eq. (5) or Eq. (6)) represents a usual LES or RANS equation depending on whether τ_L^{LES} is smaller than τ_L^{RANS} or not, respectively. The model (7) represents the simplest possible model for τ_L. The validity of this assumption will be shown in Sect. 7.2. It is worth noting that this unification approach is more general than the unification of mean velocity equations [21, 30]: by focusing the unification of methods on the scale-determining variable τ_L, the unification provides a hierarchy of deterministic models.

4. RANS-LES Coupling Approaches

The use of the time scale relation $\tau_L = min(\tau_L^{LES}, \tau_L^{RANS})$ requires the definition of τ_L^{LES} and τ_L^{RANS}. Eqs. (1) and (2) represent pure LES equations if the time scale τ_L is a linear function of the filter width Δ,

$$\tau_L^{LES} = \ell_* \tau^{LES}, \tag{8}$$

where $\ell_* = (1 \pm 0.5)/3$ and $\tau^{LES} = \Delta/k^{1/2}$, see [21]. On the other hand, Eqs. (1) and (2) represent pure RANS equations if τ_L is given by

$$\tau_L^{RANS} = 2(1 - c_o)\tau^{RANS}, \tag{9}$$

where τ^{RANS} represents the dissipation time scale of turbulence. The validity of the latter relation can be seen by using Eq. (9) in Eq. (3), which shows that the last term in Eq. (3) represents the negative dissipation rate. The model parameter c_o varies slightly depending on whether Eqs. (1) and (2) are used as LES or RANS equations. For the LES regime we have $c_o = 19/27 \approx 0.7$, and for the RANS regime we have $c_o = 0.83 \pm 0.7$, see Heinz [33]. The simulation results reported below show that the influence of such minor c_o variations is negligible. In conjunction with a theoretical reasoning [33], it is, therefore, well justified to set $\ell_* = 2(1 - c_o)$. The use of the standard value $\ell_* = 1/3$ would imply $c_o = 5/6 \approx 0.83$, which corresponds to the standard RANS value of c_o. Hence, τ_L^{RANS} can be written

$$\tau_L^{RANS} = \ell_* \tau^{RANS}. \tag{10}$$

The application of this relation requires the definition of τ^{RANS}. This question can be conveniently addressed by considering an equation for the turbulence frequence ω, which determines τ^{RANS} via the definition $\tau^{RANS} = 1/\omega$. The usual structure of the ω equation is given by

$$\frac{\widetilde{D}\omega}{\widetilde{D}t} = F\left[S^2, k, \omega, \nu, \nu_t\right], \tag{11}$$

see, for example, Eq. (17). Here, F refers to a functional of $S^2 = 2\widetilde{S}_{nk}\widetilde{S}_{nk}$, k, ω, ν, and ν_t, and the gradients of these variables in space. The turbulent viscosity $\nu_t = k\tau_L/3$ in Eq. (11) involves the time scale τ_L, which switches between the LES and RANS regimes. Instead of using Eq. (11) it would be possible to replace ν_t in (11) by the RANS limit ν_t^{RANS} in order to ensure that the ω equation provides the RANS time scale $\tau^{RANS} = 1/\omega$. However, there is no difference between this option and Eq. (11): ω is used in the unified approach only if $\tau_L = \tau_L^{RANS}$, and in that case we apply $\nu_t = \nu_t^{RANS}$ in Eq. (11).

According to Eq. (7) combined with (8) and (10), the unified time scale τ_L is given by

$$\tau_L = \ell_* min(\Delta k^{-1/2}, \tau^{RANS}) = \ell_* min(\Delta, L) k^{-1/2}, \tag{12}$$

where the characteristic time scale $L = k^{1/2}\tau^{RANS}$ of turbulence is introduced. It is relevant to note that L is not equal to the characteristic RANS length scale of large scale turbulence because the turbulent kinetic energy k is provided through the unified RANS-LES simulation. Relation (12) can be used in several ways that correspond to different coupling methods of RANS and LES equations. These coupling options will be discussed in the following three paragraphs and validated in Sect. 7.

A first approach, the exact coupling (EC) approach, is given by providing τ^{RANS} in $\tau_L = \ell_* min(\Delta k^{-1/2}, \tau^{RANS})$ by a pure RANS approach as described above. The RANS simulation is performed prior to the unified RANS-LES simulation so that the dissipation time scale τ^{RANS} is unaffected by LES. The turbulent kinetic energy k in $\tau_L = \ell_* min(\Delta k^{-1/2}, \tau^{RANS})$ is provided through the unified RANS-LES simulation. This coupling approach corresponds to the idea of providing the strict RANS limit for τ_L. Its disadvantage is the need to do a RANS simulation in addition to the unified RANS-LES simulation and to store the resulting τ^{RANS} data.

A second approach, the dynamic coupling (DC) approach, is given by providing τ^{RANS} and k in the relation $\tau_L = \ell_* min(\Delta k^{-1/2}, \tau^{RANS})$ by the unified RANS-LES simulation, which means τ^{RANS} is provided via Eq. (11) which obtains the required input from the unified RANS-LES simulation. This coupling approach corresponds to the idea of calculating the transition between RANS and LES regions dynamically as part of the unified RANS-LES simulation. This option is very attractive because it avoids the need for a separate RANS simulation, and it provides results that are (compared to the EC coupling approach) less affected by shortcomings of the RANS method applied (which are often not fully known). Thus, this option is well appropriate to study complex flows for which RANS models have not been validated or are known to fail. This coupling method has been successfully applied on the basis of the model of De Langhe et al. [31] to the prediction of turbulent swirling flows.

A third approach, the fixed coupling (FC) approach, is given by providing L in $\tau_L = \ell_* min(\Delta, L)/k^{1/2}$ by a pure RANS approach prior to the unified RANS-LES simulation, whereas the denominator $k^{1/2}$ is obtained via the unified RANS-LES method. This approach recovers the correct LES limit $\tau_L^{LES} = \Delta k^{-1/2}$ of τ_L, and it provides a RANS limit $\tau_L^{RANS} = \ell_* L/k^{1/2}$. The latter limit approximates the exact RANS limit by the assumption that $k^{1/2}$ provided by the unified model in the RANS region corresponds to $k^{1/2}$ provided by the pure RANS method. This coupling approach corresponds to the idea of fixing the transition between RANS and LES regions prior to the simulation, which may be helpful for certain flows [26]. The disadvantage of this option is the need to do a RANS simulation in addition to the unified RANS-LES simulation and to store the resulting data.

5. Linear Unified RANS-LES Model

Regarding the following developments in the first part of this two-part paper we will focus on the use of the first-order approximation (5) for D_{ij}. The second-order approximation for D_{ij} will be used in the second part of this two-part paper [85]. The flow is described by the incompressibility condition $\partial \widetilde{U}_k/\partial x_k = 0$ and the velocity equation

$$\frac{\widetilde{D}\widetilde{U}_i}{\widetilde{D}t} = -\frac{\partial(\langle p \rangle /\rho + 2k/3)}{\partial x_i} + 2\frac{\partial(\nu + \nu_t)\widetilde{S}_{ik}}{\partial x_k}. \tag{13}$$

The turbulent viscosity is given by $\nu_t = k\tau_L/3$, and the turbulent kinetic energy equation reads according Eq. (3)

$$\frac{\widetilde{D}k}{\widetilde{D}t} = -\frac{1}{2}\frac{\partial T_{knn}}{\partial x_k} + 2\frac{k\tau_L}{3}\widetilde{S}_{nk}\frac{\partial \widetilde{U}_n}{\partial x_k} - \frac{2(1-c_o)k}{\tau_L} = -\frac{1}{2}\frac{\partial T_{knn}}{\partial x_k} + 2\nu_t\widetilde{S}_{nk}\widetilde{S}_{nk} - \frac{2(1-c_o)k}{\tau_L}, \tag{14}$$

where $d_{ij}^{(1)} = -\widetilde{S}_{ij}\tau_L/3$, $\nu_t = k\tau_L/3$, and the definition of $\widetilde{S}_{nk}$ are used. This equation requires a model for the triple correlation. Such a model is given by

$$T_{knn} = -2(\nu + \nu_t)\frac{\partial k}{\partial x_k}. \tag{15}$$

The structure of this expression can be derived as a consequence of the transport equation for triple correlations, which is implied by the PDF transport equation considered [21]. This expression is extended here by the consideration of the kinematic viscosity ν. By using $S^2 = 2\widetilde{S}_{nk}\widetilde{S}_{nk}$ we can write the turbulent kinetic energy equation as

$$\frac{\widetilde{D}k}{\widetilde{D}t} = \frac{\partial}{\partial x_k}\left[(\nu + \nu_t)\frac{\partial k}{\partial x_k}\right] + \nu_t S^2 - \frac{2(1-c_o)k}{\tau_L}. \tag{16}$$

The calculation of the time scale τ_L requires the calculation of $\tau^{RANS} = 1/\omega$. To determine ω we specify the general ω equation (11) by using the model of Bredberg et al. [86],

$$\frac{\tilde{D}\omega}{\tilde{D}t} = C_{\omega 1}\frac{\omega}{k}\nu_t S^2 - \frac{C_{\omega 2}}{C_k}\omega^2 + \frac{\partial}{\partial x_j}\left[(\nu + \frac{\nu_t}{\sigma_\omega})\frac{\partial \omega}{\partial x_j}\right] + \frac{C_\omega}{k}(\nu + \nu_t)\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}. \tag{17}$$

Here, $C_{\omega 1}$, $C_{\omega 2}$, C_ω, and σ_ω are model constants that have the values

$$C_{\omega 1} = 0.49, \qquad C_{\omega 2} = 0.072, \qquad C_k = 0.09 \qquad C_\omega = 1.1, \qquad \sigma_\omega = 1.8. \tag{18}$$

The comparison with the RANS limit $\nu_t^{RANS} = \ell_* k \tau^{RANS}/3$ of ν_t used in Eqs. (16) and (17) with the RANS viscosity $\nu_t^{RANS} = C_k k/\omega$ used in the model of Bredberg et al. [86] reveals the consistency constraint

$$\ell_* = 3C_k. \tag{19}$$

Hence, the use of $C_k = 0.09$ corresponds to $\ell_* = 0.27$, which is close to the standard value $\ell_* = 1/3$ for ℓ_*, see [21]. When the ω equation is integrated through the viscous sublayer ($y^+ \leq 5$), numerical errors can distort the velocity profiles in the viscous sublayer and the log layer [19]. To avoid this problem, the value of ω at the first grid point is set explicitly using the following expression [87]

$$\omega = \sqrt{\left(\frac{2\nu}{C_k d_y^2}\right)^2 + \left(\frac{k^{0.5}}{C_k^{0.25}\kappa d_y}\right)^2}, \tag{20}$$

where $\kappa = 0.41$ and d_y is the near-wall distance. The resulting expression for ω^2 represents a combination of two terms which are used in conjunction with models that integrate to the wall (first-term) and that apply a wall function (second-term). Correspondingly, the use of Eq. (20) allows the first grid point to be located in the viscous sublayer, in the buffer layer, or in the log law region.

The turbulent viscosity $\nu_t = k\tau_L/3$ derived above does not account for the damping effect of walls on turbulent quantities. This effect can be taken into account by using the following modified turbulent viscosity ν_{t*} [2],

$$\nu_{t*} = \begin{cases} f_\mu^{LES} \nu_t^{LES} \\ f_\mu^{RANS} \nu_t^{RANS} \end{cases}. \tag{21}$$

Here, ν_t^{LES} refers to the turbulent viscosity in the LES limit, and f_μ^{LES} and f_μ^{RANS} are damping functions in the LES and RANS limits, respectively. For the LES damping function f_μ^{LES} we use an expression proposed by Kajishima and Nomachi [88],

$$f_\mu^{LES} = \frac{\Delta}{1 + c_k \Delta^2 S^2/k}, \tag{22}$$

where $c_k = 0.08$. For the RANS damping function f_μ^{RANS} we use an expression applied in conjunction with the model of Bredberg et al. [86],

$$f_\mu^{RANS} = 0.09 + \left(0.91 + \frac{1}{Re_t^3}\right)\left(1 - e^{-(Re_t/25)^{2.75}}\right). \tag{23}$$

Here, Re_t is the turbulence Reynolds number, which is defined by $Re_t = C_k k/(\omega\nu)$. These expressions f_μ^{LES} and f_μ^{RANS} ensure the correct scaling $O(y^3)$ of the turbulent viscosity in the near-wall region: by using a Taylor series expansion [19, 86] we find in the LES limit $\nu_t^{LES} \sim O(y)$ and $f_\mu^{LES} \sim O(y^2)$, and in the RANS limit we find $\nu_t^{RANS} \sim O(y^4)$ and $f_\mu^{RANS} \sim O(1/y)$.

The last term in Eq. (16) represents the negative dissipation rate, this means we have $\epsilon = 2(1 - c_0)k/\tau_L$. The scaling of ϵ in the near-wall region requires attention, too. The dissipation rate should scale as $\epsilon \sim y^0$ in the near-wall region. In the RANS limit, the dissipation rate shows the correct scaling in the near-wall region [86]. However, in the LES limit we have $\epsilon^{LES} \sim O(y^3)$. A way to overcome this problem is to use a modified dissipation rate $\epsilon_*^{LES} = \epsilon^{LES} + \epsilon_w$ in the LES limit, where ϵ_w is given by [88]

$$\epsilon_w = 2\nu \frac{\partial \sqrt{k}}{\partial x_j} \frac{\partial \sqrt{k}}{\partial x_j}. \tag{24}$$

The consideration of ϵ_w, which is characterized by $\epsilon_w \sim O(y^0)$, ensures the correct asymptotic behavior $\epsilon \sim y^0$ of the dissipation rate in the near-wall region.

6. Numerical Method

The sketch of the computational domain is shown in Fig. 1. The domain size ($L_x * L_y * L_z$) depends on the friction Reynolds number $Re_\tau = u_\tau \delta/\nu$. Here, $u_\tau = \sqrt{\tau_w/\rho}$ is the friction velocity, τ_w is the wall shear stress, δ is the half channel width, and ν is the kinematic viscosity. The unified simulations were performed using the same code, whereas the DNS simulations were performed using a different code.

DNS calculations have been performed using an incompressible Navier-Stokes solver [89, 90]. The algorithm employs spectral discretization (Fourier modes along the periodic directions and Chebyshev polynomials along the wall normal direction) for the spatial derivatives. The convection term was formulated in the skew-symmetric form to avoid aliasing errors. It has been computed explicitly. The viscous term was treated implicitly. Time marching was performed using a fourth-order backward difference scheme. The pressure gradient that drives the flow in the channel has been adjusted dynamically to maintain a constant mass flow rate. Periodic boundary conditions were employed along the streamwise (x) and spanwise (z) direction while a no slip boundary condition has been employed along the wall normal direction (y). The time step was modified dynamically to ensure a constant CFL number of 0.5. The total time of simulation was $t = 320\,\delta/u_\tau$. A time period of approximately $t = 100\,\delta/u_\tau$ was used for the calculation of the flow development. The statistics were then taken over a time period $t = 220\,\delta/u_\tau$. The DNS computations were performed using the spectral code for $Re_\tau = 395$ corresponding to a Reynolds number $Re = U_b L_y/\nu = 13350$, where U_b refers to the bulk velocity. The domain size was $2\pi * 2 * \pi$, and the grid applied was $256 * 193 * 192$ [91].

The unified RANS-LES models have been implemented in the OpenFOAM CFD Toolbox [87]. The calculations have been performed using a finite-volume based method with the numerical grid being used as the LES filter. The convection term was discretized using a second-order central difference scheme in the momentum equation and a bounded second-order central difference scheme in the turbulence transport equations to ensure a stable solution. All other terms were discretized using a second-order central difference scheme. The pressure gradient that drives the flow in the channel has been adjusted dynamically to maintain a constant mass flow rate. PISO algorithm was used for the pressure-velocity coupling [92]. The resulting algebraic equations for all the flow variables except the pressure have been solved iteratively using a preconditioned biconjugate gradient method with a diagonally incomplete LU preconditioning at each time step. The Poisson equation for the pressure was solved using an algebraic multigrid (AMG) solver. When the scaled residual became less than 10^{-6}, the algebraic equations were considered to be converged. Time marching was performed using a second-order backward difference scheme. The time step was modified dynamically to ensure a constant CFL number of 0.5. Periodic boundary conditions have been employed along the streamwise and spanwise directions for all the flow variables. Along the wall normal direction, a no slip boundary condition was used for velocity and the modeled turbulent kinetic energy was set to zero. For ω, Eq. (20) was used at the first near-wall grid point as the boundary condition. Unified RANS-LES simulations at a friction Reynolds number $Re_\tau = 395$ were used for the investigations reported in the first part of this two-part paper. The simulations have been performed on many different grids, which are given in Table 1. A simulation time $t = 100\,\delta/u_\tau$ was used to eliminate the effect of the initial conditions. Statistics were then taken over $t = 220\,\delta/u_\tau$.

The results reported in the following sections require the calculation of different ensemble averaged and filtered variables. The calculation of these variables from DNS data is explained here. The ensemble mean $\langle F\rangle_e$ of any variable F is calculated by

$$\langle F\rangle_e = \frac{1}{N_t N_x N_z}\sum_{i=1}^{N_t}\sum_{j=1}^{N_x}\sum_{k=1}^{N_z} F_{ijk}(x,y,z,t). \tag{25}$$

Here, N_t is the number of temporal samples used for the averaging, and N_x and N_z are number of points in the streamwise and spanwise directions, respectively. The analysis of the DNS data showed that there was a very little difference between the cases $N_t = 1$ and $N_t > 1$. Hence, all the analyses were performed by setting $N_t = 1$. The ensemble mean of the instantaneous velocity field was calculated using Eq. (25). The ensemble means of the turbulent kinetic energy and dissipation rate were calculated from the ensemble mean of the velocity and its gradients using the expressions

$$k^{RANS} = 0.5\left[\langle U_i U_i\rangle_e - \langle U_i\rangle_e \langle U_i\rangle_e\right], \qquad \epsilon^{RANS} = 2\nu\left[\langle S_{ij} S_{ij}\rangle_e - \langle S_{ij}\rangle_e \langle S_{ij}\rangle_e\right]. \tag{26}$$

Assuming a box filter, the filtered value $\widetilde{F}$ of any variable F is calculated by

$$\widetilde{F}(x,y,z,t) = \frac{1}{\Delta_x \Delta_z}\int_{x-\Delta_x/2}^{x+\Delta_x/2}\int_{z-\Delta_z/2}^{z+\Delta_z/2} F(x,y,z,t)\,dxdydz. \tag{27}$$

The trapezoidal rule is used for the integration. The integration is not performed along the wall-normal direction because of the non-uniformity of the grid. The magnitude of the streamwise and spanwise spacing Δ_x and Δ_z was varied in the following way: $\Delta_x^{DNS} \le \Delta_x \le 20\Delta_x^{DNS}$ and $\Delta_z^{DNS} \le \Delta_z \le 20\Delta_z^{DNS}$, respectively. The filtered velocity field was calculated using Eq. (27). The kinetic energy and dissipation rate are calculated from the filtered instantaneous velocity field $\widetilde{U}$ and its gradient as follows,

$$k = 0.5(\widetilde{U_i U_i} - \widetilde{U_i}\widetilde{U_i}), \qquad \epsilon = 2\nu(\widetilde{S_{ij} S_{ij}} - \widetilde{S_{ij}}\widetilde{S_{ij}}). \tag{28}$$

It is worth noting that k and ϵ obtained in this way represent unified variables: depending on the filter width applied they range from LES variables to RANS variables. All the results shown below have been averaged along the homogeneous directions.

7. Analysis of Coupling Approaches

In Sect. 4, the unification of RANS and LES equations was achieved by defining the unified time scale as $\tau_L = \ell_* min(\tau^{LES}, \tau^{RANS})$. This assumption leads to three relevant questions. The first question is how the filter width Δ in $\tau^{LES} = \Delta/k^{1/2}$ should be defined. According to $\tau_L = \ell_* min(\tau^{LES}, \tau^{RANS})$, the filter width Δ determines the location of the RANS-LES interface, which has a significant effect on the predictions of the unified model [85]. The second question is about the suitability of switching between RANS and LES according to the definition $\tau_L = \ell_* min(\tau^{LES}, \tau^{RANS})$. The latter choice is the simplest possible assumption, and the question is whether other ways for performing the transition between RANS and LES are more appropriate. The third question is about the most appropriate way to provide τ^{RANS}, which is the question about the most appropriate coupling approach. This question definitely has an influence on the computational efficiency, see the discussion of coupling approaches and their computational consequences in Sect. 4. These three questions will be addressed in the following three subsections, respectively. To obtain the required instantaneous data (which are unavailable), this will be done by means of DNS performed for the $Re_\tau = 395$ case. Such simulations are computationally efficient and sufficient for significantly reducing the influence of Reynolds number effects.

7.1. Choice of Filter Width

A variety of definitions of the filter width have been used for hybrid RANS-LES simulations on structured grids: the geometric mean of a cell, $\Delta = (\Delta_x \Delta_y \Delta_z)^{1/3}$ [2], the smallest side of a cell, $\Delta = \min(\Delta_x, \Delta_y, \Delta_z)$ [37], the maximum area of cell faces, $\Delta = (\max(\Delta_x\Delta_y, \Delta_x\Delta_z, \Delta_y\Delta_z))^{1/2}$ [93], and the large side of a cell, $\Delta = \max(\Delta_x, \Delta_y, \Delta_z)$ [52]. An advantage of the geometric mean and face area filter width is that these filters can be used in a straightforward way on unstructured and hybrid grids. To account for the grid anisotropy, these filter width definitions were considered by multiplying the filter width definition with the anisotropy function [94]

$$f(a_1, a_2) = \cosh \sqrt{4\left[(\ln(a_1) - \ln(a_2))^2 + \ln(a_1)\ln(a_2)\right]/27}. \tag{29}$$

We use here $a_1 = \Delta_1/\max(\Delta_x, \Delta_y, \Delta_z)$ and $a_2 = \Delta_2/\max(\Delta_x, \Delta_y, \Delta_z)$, where Δ_1 and Δ_2 represent the two cell sides that are smaller than $\max(\Delta_x, \Delta_y, \Delta_z)$. The variation of the filter width according to these four choices was calculated by using the DNS-RANS grid. The results are shown along the wall-normal direction (the grid spacing is constant along the streamwise and spanwise directions) in Fig. 2. This figure shows that there are significant differences between the filter width definitions. The small side filter gives the minimum value for the filter width, and the large side filter gives the maximum value. The face area filter width is slightly smaller than the large side filter width, while the geometric mean width has almost the half of the value of the large side filter width. Such differences will vary with the grid refinement or coarsening. However, the small side filter width will be not affected because $\Delta_y \ll (\Delta_x, \Delta_z)$ in wall-bounded flow simulations.

The suitability of different filter width definitions can be studied by considering the corresponding implications for the LES-RANS transition. By coarsening the grid, the unified method will switch from LES to RANS if the grid becomes very coarse. For such a very coarse grid, the unified time scale $\tau_L = min(\tau_L^{LES}, \tau_L^{RANS})$ has to provide τ_L^{RANS} for all definitions of Δ, which requires that $\tau_{LES} > \tau_{RANS}$ everywhere in the domain. The LES time scale is always given by $\tau^{LES} = \Delta k^{-1/2}$. We combine the investigation of this question with the consideration of the suitability of the three coupling approaches discussed in Sect. 4, this means the RANS time scale will be defined as

$$\tau_{EC}^{RANS} = \frac{k^{RANS}}{\epsilon^{RANS}}, \qquad \tau_{DC}^{RANS} = \frac{k}{\epsilon}, \qquad \tau_{FC}^{RANS} = \frac{k^{RANS}}{\epsilon^{RANS}}\sqrt{\frac{k^{RANS}}{k}}. \tag{30}$$

The corresponding values of k and ϵ are defined by the relations (26) and (28). It is worth emphasizing that the choice of the coupling approach may have a significant effect on the definition of the τ_{RANS}. The latter fact is shown in Fig. 3, which shows $\tau_{DC}^{RANS}/\tau_{EC}^{RANS}$ and $\tau_{FC}^{RANS}/\tau_{EC}^{RANS}$ for four different grids. This figure does also show that both τ_{DC}^{RANS} and τ_{FC}^{RANS} converge to τ_{EC}^{RANS} with increasing grid coarsening, as required by the definition of these time scales.

The question of whether all filter width definitions satisfy the requirement described in the preceding paragraph will be considered by using the DNS - RANS grid for which $\Delta_x = 20\Delta_x^{DNS}$, $\Delta_y = \Delta_y^{DNS}$, and $\Delta_z = 20\Delta_z^{DNS}$. This grid is very coarse along the streamwise and spanwise directions. As may be seen in Fig. 3, τ_{DC}^{RANS} and τ_{FC}^{RANS} are very close to τ_{EC}^{RANS}. Thus, for this grid, the unified model should provide the RANS limit everywhere in the domain. The plots of LES and RANS time scales (given in seconds) for the EC, DC and FC approaches are shown in Figs. 4a-d for the small side, geometric mean, face area and large side filter width definitions, respectively. These results show that the small side and geometric filter width definitions are inappropriate because they cause the LES time scale to be smaller than the RANS time scale. Their use would imply LES regions in the flow field on this very coarse grid, which results in erroneous predictions because LES calculations become inaccurate on coarse grids [85]. Regarding the large side filter, the requirement $\tau_{LES} > \tau_{RANS}$ is satisfied by all the coupling approaches, but for the face area filter, $\tau_{LES} > \tau_{RANS}$ is not satisfied for the FC approach. Consequently, the large side filter will be applied in the following. This approach is also well appropriate for comparisons with other hybrid RANS-LES methods like DES, which usually apply the large side filter [26].

7.2. Choice of Transfer Function

In Sect. 4 we introduced the model $\tau_L = \ell_* min(R_\tau, 1)\tau^{RANS}$ for the unified time scale, where we introduced the time scale ratio $R_\tau = \tau^{LES}/\tau^{RANS}$. Here, $\tau^{LES} = \Delta k^{-1/2}$, and the definition of τ^{RANS} depends on the coupling approach applied (see Sect. 4). The model $\tau_L = \ell_* min(R_\tau, 1)\tau^{RANS}$ is the simplest possible choice, so let us have a closer look at its suitability. For doing this we rewrite the time scale model in the following way. The last term in Eq. (14) shows that the unified dissipation rate is given by $\epsilon = \ell_* k/\tau_L$, where $\ell_* = 2(1 - c_o)$ is used. Hence, the unified Lagrangian time scale is given by $\tau_L = \ell_* \tau$, where $\tau = k/\epsilon$ represents the unified dissipation time scale. Correspondingly, the unified time scale model $\tau_L = \ell_* min(R_\tau, 1)\tau^{RANS}$ implies that $\tau = min(R_\tau, 1)\tau^{RANS}$. By introducing the transfer function $T(R_\tau) = \tau/\tau^{RANS}$, the claim made in Sect. 4 is that we can use the model $T(R_\tau) = min(R_\tau, 1)$ for the transfer function.

The claim $T(R_\tau) = min(R_\tau, 1)$ can be proven by comparing $T(R_\tau)$ models with DNS calculations of $T(R_\tau)$. Due to its definition $T(R_\tau) = \tau/\tau^{RANS}$, the transfer function can be calculated from DNS data by the expression

$$T(R_\tau) = \frac{k/\epsilon}{k_{RANS}/\epsilon_{RANS}}. \tag{31}$$

The values of k_{RANS} and ϵ_{RANS} follow from the relations (26), and the values of k and ϵ follow from the relations (28). A reasonable model for the transfer function $T(R_\tau)$ is given by [33]

$$T(R_\tau) = \frac{1}{2}R_\tau - \frac{\lambda}{2}\ln\left[\frac{\cosh((1-R_\tau)/\lambda)}{\cosh(1/\lambda)}\right]. \tag{32}$$

In difference to the expression $T(R_\tau) = min(R_\tau, 1)$ used before, this model provides a smooth transition between R_τ and one. For λ = 0, we find that $T(R_\tau) = min(R_\tau, 1)$. The suitability of this model and the optimal setting of the smoothing parameter λ will be considered in the following regarding the EC, DC, and FC coupling approaches. Hence, the model function (32) will be considered in dependence on $R_\tau = \tau^{LES}/\tau^{RANS}_{EC}$, $R_\tau = \tau^{LES}/\tau^{RANS}_{DC}$, and $R_\tau = \tau^{LES}/\tau^{RANS}_{FC}$ for the EC, DC, and FC coupling approaches, respectively. Here, the RANS time scales involved are calculated according to the relations (30).

The comparison between the exact transfer function (31) and model transfer function (32) is shown in the Figs. 5, 6, and 7 for the EC, DC, and FC approach, respectively. The model transfer function (32) is plotted for three different λ values ($0,\ 0.25,$ and 0.5). It can be seen that the model tranfer function of all three coupling approaches provides for the different values of λ a good model for the exact transfer function. To determine an optimal value of λ, the error between the exact and model transfer functions is shown in Figs. 5, 6, and 7 regarding the DNS-C grid, which is typically used for channel flow simulation with hybrid RANS-LES methods. The error was calculated as

$$E_\lambda = 100\sqrt{\sum_{i=1}^{N}(T_i^E - T_i^M)^2}\Big/\sqrt{\sum_{i=1}^{N}(T_i^E)^2}, \tag{33}$$

where T_i^E and T_i^M refer to the exact and model transfer function values, respectively, at the grid point considered. For the EC, DC, and FC coupling approaches the error was found to be minimal for $\lambda = (0.23, 0.2, 0.2)$, respectively. The differences between the use of the latter λ values and the use of $\lambda = 0$ were found to be negligible in simulations: the effects on the mean velocity and stresses were below 0.02%. Thus, all further simulations have been performed for $\lambda = 0$.

7.3. Choice of Coupling Approach

The third question addressed in this section concerns the suitability of coupling approaches. Fig. 8 shows the RANS time scales for the three coupling approaches considered on four different grids: DNS - F, DNS - R, DNS - C and DNS - RANS. The corresponding LES time scales are also shown for a comparison. It may be seen that τ^{RANS}_{EC} is unaffected by the grid applied, as required by the definition of this time scale. Regarding τ^{RANS}_{DC} we observe minor variations with the grid, whereas τ^{RANS}_{FC} is strongly affected by the grid. This fact indicates that the use of the FC coupling approach is less appropriate than the use of the EC and DC coupling approaches.

Further inside into this question can be obtained by considering the transfer function $T(R_\tau) = min(R_\tau, 1)$ for the three coupling approaches on the grids considered in Fig. 8. The corresponding plots are presented in Fig. 9. The value of the transfer function shows in which flow regions RANS and LES are applied: RANS simulations are performed if $T = 1$, and LES is performed for $T < 1$. It may be seen that (outside the viscous region) there is no difference between the coupling approaches for the DNS - F and DNS - RANS grids: all coupling approaches correspond to LES and RANS simulations, respectively. Differences between the coupling approaches may be seen for the DNS - R and DNS - C grids, for which all coupling approaches involve both RANS and LES regions. As required, the RANS region becomes more extended with a growing grid coarsening. A relevant conclusion is that the DC approach provides the largest RANS region among the coupling approaches. This is a desired feature because previous studies with hybrid RANS-LES models showed that the simulation results improve with a growing distance of the RANS - LES interface from the wall [55]. Correspondingly, the DC coupling approach will be used in the following.

8. Model Properties Evaluation

In the last paragraph of Sect. 3 it was argued that the unified RANS-LES models presented here satisfy the properties P1, P2, and P3 of an optimal hybrid RANS-LES model, which were formulated in the beginning of Sect. 3. Some specific questions related to these model properties will be addressed in the following. These analyses were performed by applying the linear unified model in simulations at $Re_\tau = 395$.

8.1. Realizability

The conclusion obtained in Sect. 3 that the unified RANS-LES models considered satisfy the realizability constraint is a consequence of the fact that the RANS-LES equations were derived as a consequence of a realizable stochastic turbulence model. However, there is also another notion of realizability focusing directly on the properties of the stress tensor. This realizability condition requires that the stress tensor is non-negative definite, as required by its definition. According to Schumann [82], the Reynolds stress tensor satisfies this condition if the three principal invariants $I_1 = D_{ii}$, $I_2 = D_{ii}D_{jj} - (D_{ij})^2$ and $I_3 = det(D_{ij})$ of the stress tensor have non-negative values. Vreman et al. [80] considered the same question regarding the SGS stress tensor. They showed that the SGS stress tensor has to satisfy the same realizability conditions as the Reynolds stress tensor. In addition, the non-negativeness of the spatial filter function, $G(\vec{r}) \geq 0$, for all $\vec{r}$ was found to be required to ensure the realizability of SGS stress tensor. It is worth noting that the derivation of turbulence models from an underlying stochastic model in general cannot ensure that the stress tensor is non-negative definite. Apart from that, the use of empirical damping functions in the near-wall region and numerical errors in simulations may imply that the model is non-realizable [95].

The realizability of the linear unified model was investigated over a wide range of grid sizes by calculating the three principal invariants I_1, I_2, and I_3 of the unified stress tensor, where $D_{ij} = D_{ij}^{(1)}$. The calculation followed the analysis of Fureby and Tabor [95]. For each simulation, ten time steps were selected at instants well separated in time (the time interval was $100\,\delta/u_\tau$) so that they can be considered statistically independent. The principal invariants I_1, I_2, and I_3 were calculated as averages over these times. The number of grid points and the percentage of grid points at which the realizability conditions were violated are shown in Table 2 for the different grids considered. Realizability constraint violations were observed only for the VCLES and CLES grids. The values of invariants were of the order of $I_1, I_2, I_3 \sim -10^{-9}$ at the grid points at which the violation occurred. Correspondingly, these violations are of the order of numerical errors in simulations and not due to the unified model.

8.2. Limits of the Unified Model

The unified RANS-LES models introduced in Sect. 3 (which correspond to the use of the EC coupling approach) describe continuous variations between the DNS, LES and RANS scale. After developing a corresponding computational method for the linear unified RANS-LES model in following sections, there is the question of how the DNS and RANS limits are realized by the computational method. Regarding the large Δ limit there is the question of whether the computational method applying the DC coupling approach results in a RANS method for a large filter width Δ. Regarding the small Δ limit there is the question of how the DNS limit is realized. In particular, there is the question of whether the DNS scaling obtained with the filter width Δ defined by the large side filter provides a DNS scaling in consistency with theoretical analyses [96]. These questions about the limits of the computational method will be addressed here regarding the use of the linear unified RANS-LES model in simulations.

The transition from DNS to the LES and RANS scales is illustrated in Fig. 10 which shows the ratio $r_k = k/(k + k_{res})$ of the modeled turbulent kinetic energy to the total kinetic energy along the wall-normal direction, where k_{res} refers to the resolved turbulent kinetic energy. Hence, the DNS limit ($r_k = 0$) and RANS limit ($r_k = 1$) are obtained everywhere in the domain if the grid is sufficiently fine or coarse, respectively. However, on fine grids there will be a difference between the filtered velocity $\widetilde{U}$ obtained from the unified simulation and the velocity field U obtained from DNS without using any turbulence model. Correspondingly, on coarse grids there will be a difference between $\widetilde{U}$ obtained from a unified simulation and the mean velocity obtained by using a pure RANS model. These differences depend on r_k. An empirical expression which provides a relation between Δ and r_k is a useful tool for the construction of grids for unified simulations. For example, such a relation can be used to account for grid requirements in certain flow regions (e.g., to ensure that LES is performed in a transitional flow region). The variation of the peak value r_{kp} of r_k with the filter width Δ is shown in Fig. 11. Here, r_k was calculated as in Fig. 10 by considering the anisotropy function (29). The value of Δ refers to the maximum of Δ provided by the large side filter without using the anisotropy function. Thus, there is one Δ value per grid. The following exponential fit is considered to quantify the variation of r_{kp} with the filter width Δ,

$$r_{kp} = \left[1 - \exp\left(-\alpha \Delta^{\beta}\right)\right]^{4/\beta}, \tag{34}$$

where α and β are model constants. This equation structure ensures that we recover $r_{kp} \sim \Delta^4$ in the small-Δ limit in agreement with the corresponding theoretical estimate obtained by Pope [96]. The values of the constants were calculated by minimizing the error between the r_{kp} values observed in simulations and the corresponding r_{kp} values calculated by means of Eq. (34). The minimal L2 error was found to be 0.027% for the values $\alpha = 4.84$ and $\beta = 0.53$. The comparison between the simulation data and the numerical fit (34) is shown in Fig. 11. It can be seen that the empirical fit provides a very good approximation to the data over the entire range of r_{kp} values.

9. Summary

The motivation of the introduction of hybrid RANS-LES methods is a computational cost reduction of LES by orders of magnitudes. However, a huge variety of hybrid RANS-LES models are currently in use such that there is the question of which hybrid RANS-LES method represents the optimal approach. This question matters because there are significant accuracy and cost differences between different hybrid RANS-LES methods [27].

The properties of an optimal hybrid RANS-LES model were formulated here by taking reference to fundamental properties of fluid flow equations. It was shown that the unified RANS-LES models derived from an underlying stochastic turbulence model [33] have the properties of an optimal hybrid RANS-LES model. The computational efficiency of unified RANS-LES models depends significantly on the way in which RANS and LES equations are coupled. The suitability of three coupling methods was investigated here regarding the linear unified RANS-LES model by *a-priori* analyses of channel flow data. It was shown that the DC coupling approach, which uses RANS and LES equations dynamically, represents the most convenient approach. The coupling analyses were also used to computationally fully develop unified RANS-LES methods by determining the most appropriate filter width and transfer function definitions. *A-posteriori* analyses of channel flow data were used then to demonstrate that the computational model obtained in this way does also satisfy the properties of an optimal hybrid RANS-LES model. It was shown that the stress tensor of the linear unified RANS-LES model satisfies the realizability requirement to be non-negative definite. It was also shown that the linear unified RANS-LES model varies continuously between the DNS, LES, and RANS limits. The influence of choosing the computational grid on the (DNS, LES, and RANS) nature of the model applied was specified in terms of scaling relation (34). It is worth noting that the numerical implementation of the unified RANS-LES model is straightforward and requires only minor modification of existing methods.

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Number	Grid Name	Grid size
1.	DNS-F	$128 * 193 * 96$
2.	DNS-R	$64 * 193 * 48$
3.	DNS-C	$32 * 193 * 24$
4.	DNS-RANS	$8 * 193 * 4$
5.	RANS	$2 * 64 * 2$
6.	VVVCLES	$4 * 64 * 4$
7.	VVCLES	$8 * 64 * 8$
8.	VCLES	$16 * 64 * 16$
9.	CLES	$32 * 64 * 32$
10.	LES	$64 * 64 * 64$
11.	FLES	$64 * 100 * 64$

Table 1: Grid nomenclature. The first four grids are used for *a-priori* analyses: F, R, and C refer to fine, regular, and coarse LES grids, respectively, and RANS refers to a RANS grid. A wall-normal (y) filtering is not applied because the grid spacing is non-uniform (such filtering can introduce numerical errors). The remaining grids are used for *a-posteriori* analyses (unified simulations), see Sect. 8. FLES refers to a fine LES grid. The other grids have the same wall-normal spacing due to the wall-normal refinement required for the RANS region. The notation VVVC, VVC and VC refers to very very very coarse, very very coarse, and very coarse LES grids.

Grid	I_1 Violation		I_2 Violation		I_3 Violation	
	Number of Points	Percent	Number of Points	Percent	Number of Points	Percent
RANS	0	0	0	0	0	0
VVVCLES	0	0	0	0	0	0
VVCLES	0	0	0	0	0	0
VCLES	7	0.042	18	0.11	16	0.098
CLES	13	0.02	47	0.072	51	0.078
LES	0	0	0	0	0	0
FLES	0	0	0	0	0	0

Table 2: Realizability analysis of the linear unified stress tensor for the $Re_\tau = 395$ case. I_1, I_2, and I_3 refer to the three principal invariants of the turbulent stress tensor (see Sect. 8.1). The grids considered are defined in Table 1. At a given grid point, a violation refers to the occurrence of a negative value of an invariant.

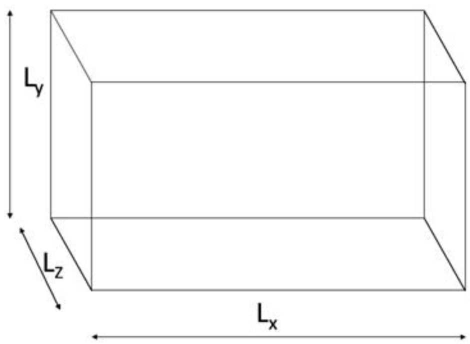


Figure 1: Problem setup: The domain size is $2\pi * 2 * \pi$ for the $Re_\tau = 395$ case considered.

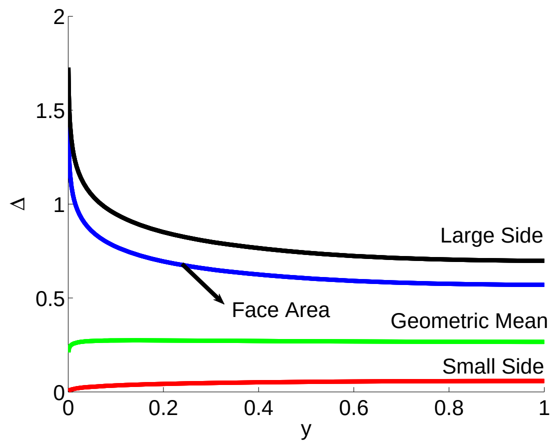


Figure 2: The variation of the filter width Δ along the wall-normal direction y for four filter width definitions.

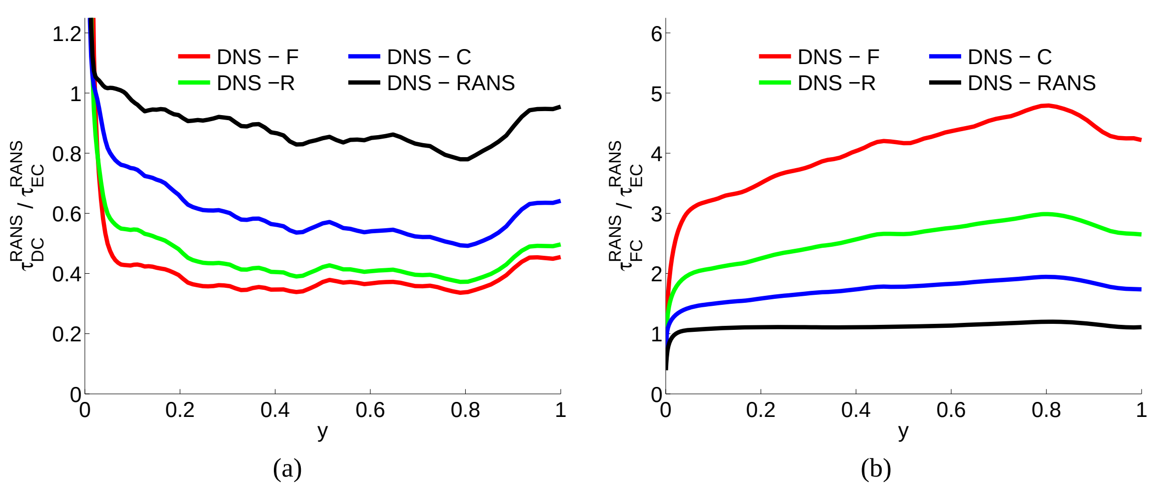
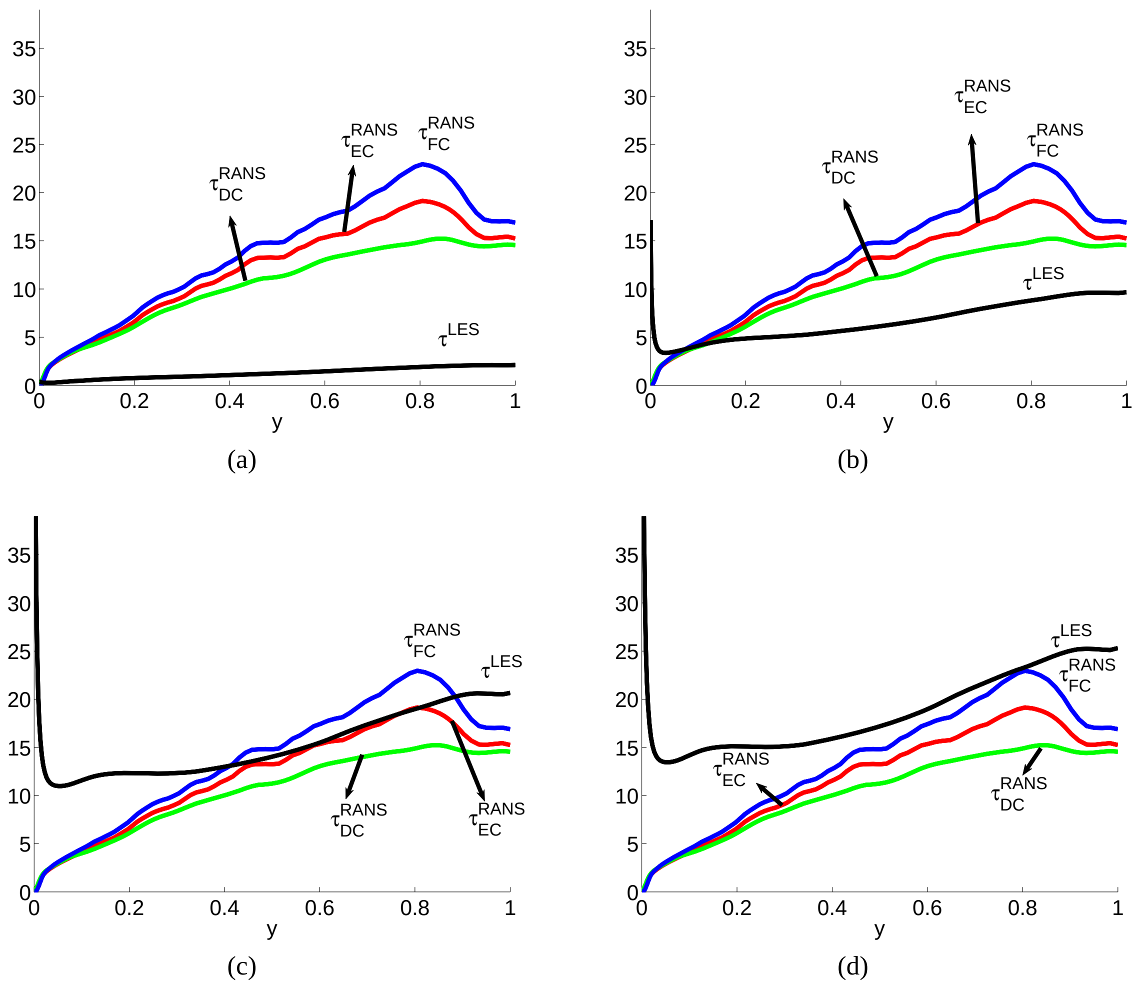


Figure 3: Ratio of time scales in the DC and FC approach to the exact RANS time scale obtained from *a-priori* analyses: (a) dynamic coupling, and (b) fixed coupling.



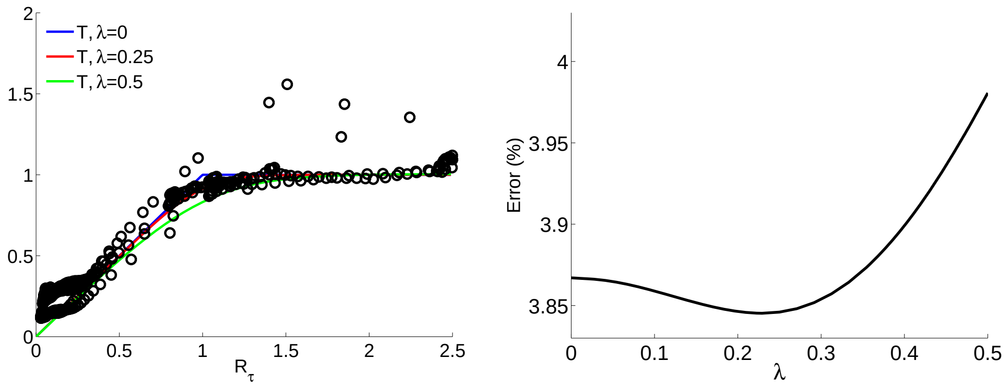
(a)

(b)

(c)

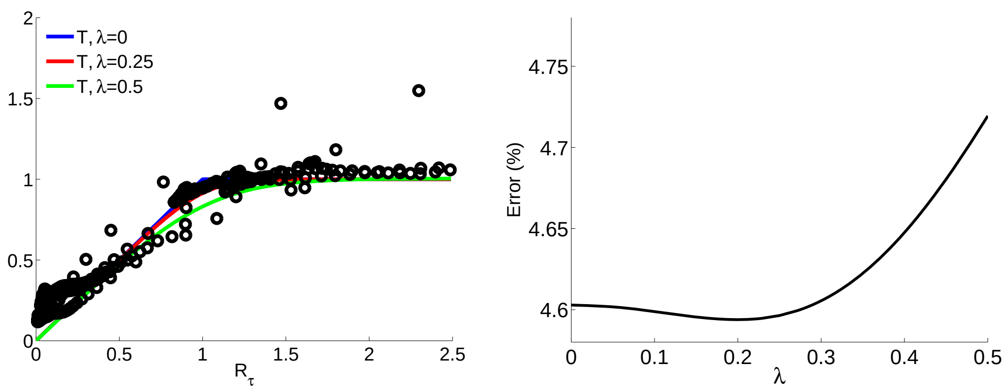
(d)

Figure 4: *A-priori* analysis results for RANS and LES time scales obtained for the EC, DC, and FC coupling approaches on the DNS-RANS grid. The following filter width definitions are applied: (a) Small side filter, (b) Geometric mean filter, (c) Face area filter, and (d) Large side filter.



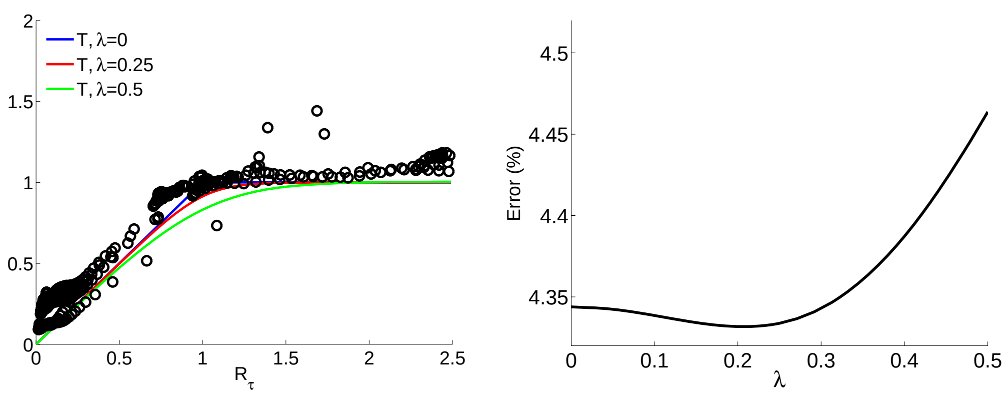
(a) (b)

Figure 5: Transfer function in the EC approach: (a) The exact transfer function (31) obtained from DNS is shown by dots, and the model transfer function (32) is shown by lines for three λ values; (b) The error (33) between the exact transfer function and the model transfer function using different λ values.



(a) (b)

Figure 6: The DC coupling approach results in correspondence to Fig. 5.



(a) (b)

Figure 7: The FC coupling approach results in correspondence to Fig. 5.

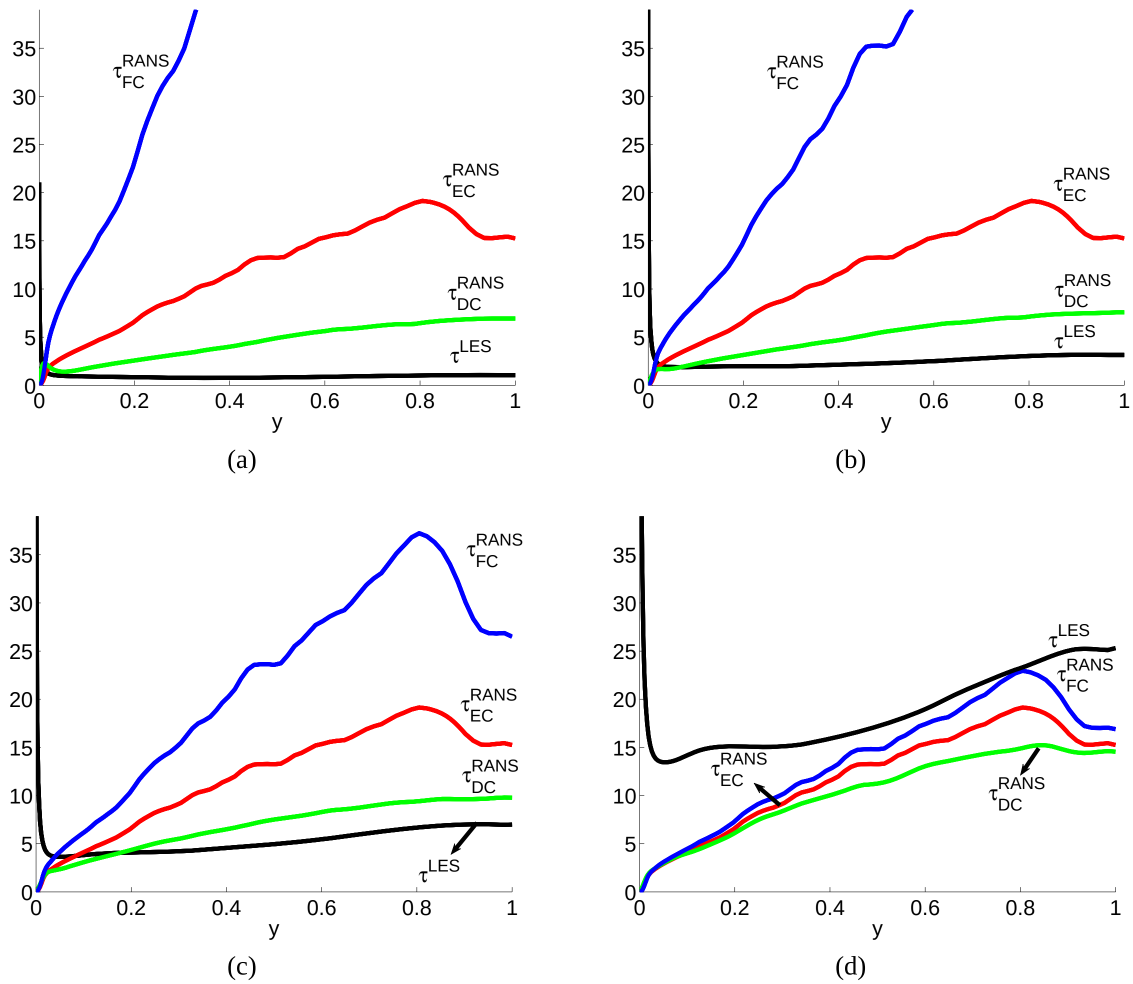


Figure 8: *A-priori* analysis results for RANS and LES time scales obtained for the EC, DC, and FC coupling approaches on different grids: (a) DNS - F grid, (b) DNS - R grid, (c) DNS - C grid, and (d) DNS - RANS grid.

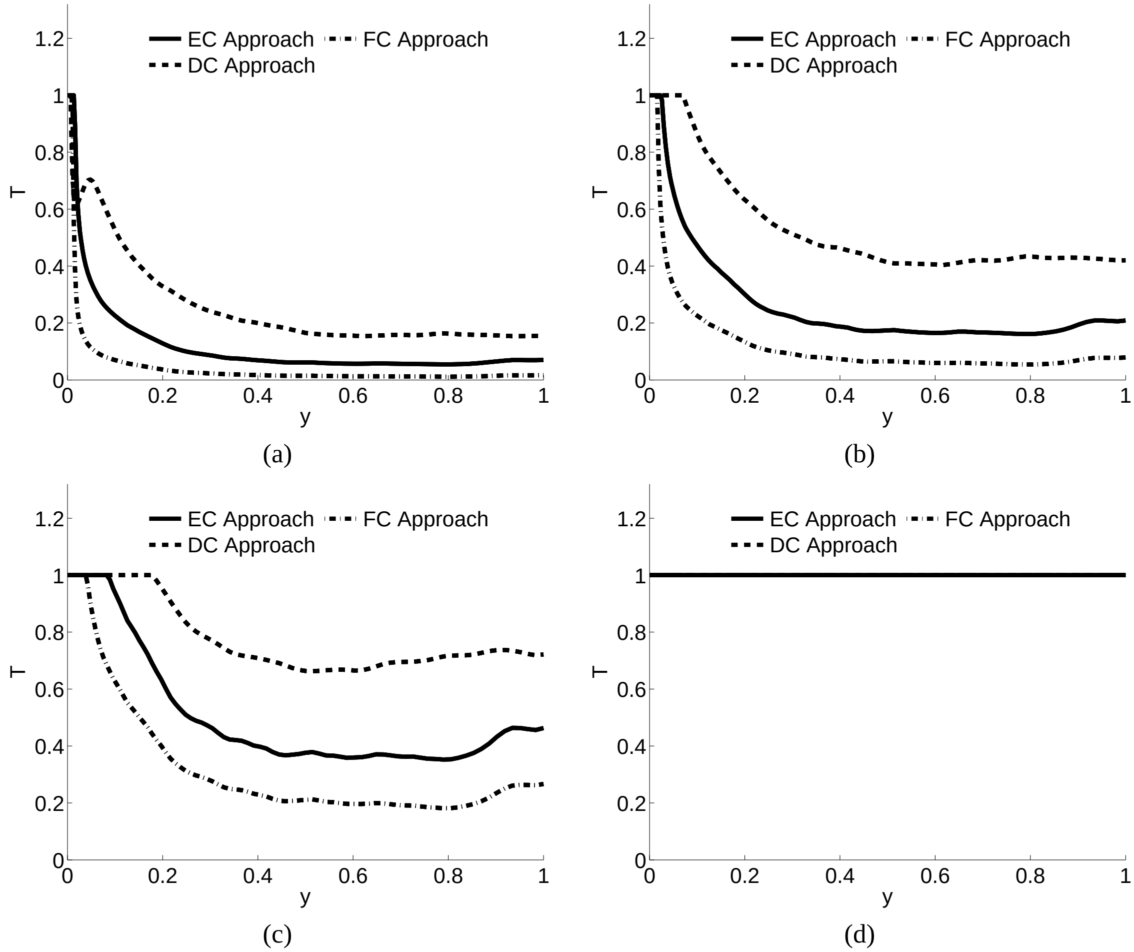


Figure 9: *A-priori* analysis results for the transfer function obtained for the EC, DC, and FC coupling approaches on different grids: (a) DNS - F grid, (b) DNS - R grid, (c) DNS - C grid, and (d) DNS - RANS grid.

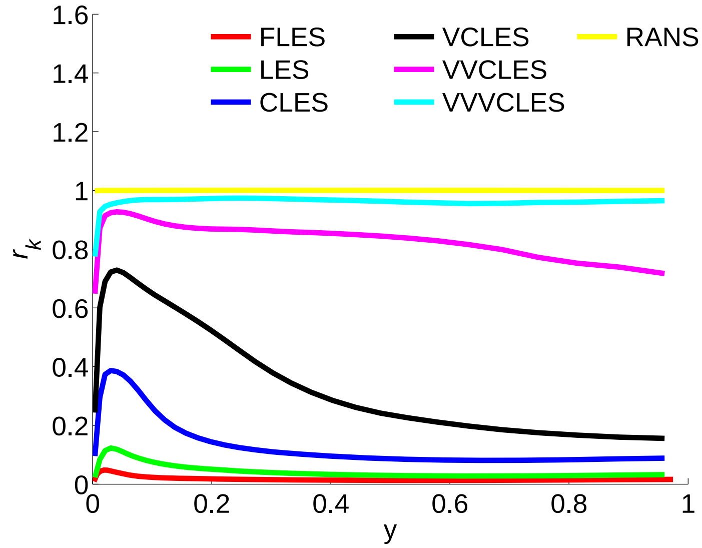


Figure 10: The ratio $r_k = k/(k + k_{res})$ of the modeled turbulent kinetic energy k to the total turbulent kinetic energy along the wall-normal direction y obtained from unified simulations on different grids. Here, k_{res} refers to the resolved turbulent kinetic energy.

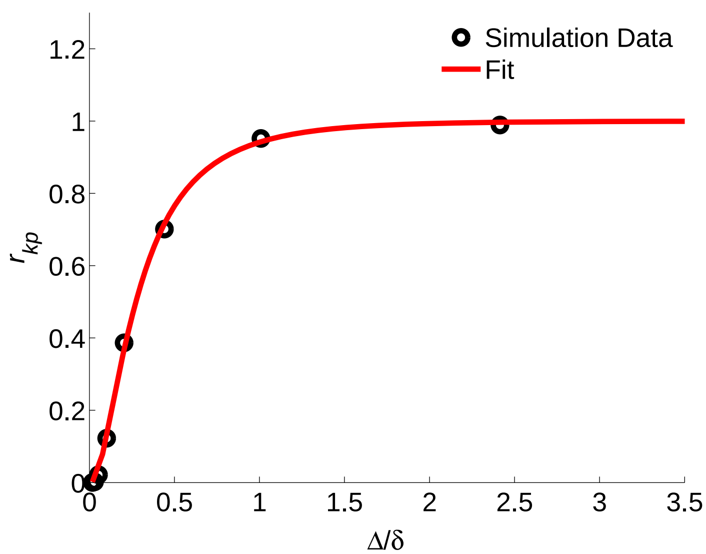


Figure 11: The dots show the peak value r_{kp} of the r_k curves given in Fig. 10 in dependence on the grid applied (Δ/δ). The line shows Eq. 34.