Scrutinizing Velocity and Pressure Coupling Conditions for LES with Downstream RANS Calculations

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Abstract

A RANS calculation is connected to an upstream LES via explicit coupling conditions at a pre-defined interface. The role of the interface is to allow for mean flow information to propagate upstream and for fluctuations to leave the LES domain without reflections. To this end, the mean velocity is directly coupled across the domain boundaries whereas the fluctuations at the downstream end of the LES zone are treated using either the so-called *enrichment* strategy (Quéméré & Sagaut, 2002) or a parameter-free generalization of this method based on a convective condition (von Terzi, Fröhlich & Mary, 2006). For incompressible flows, both techniques require a complementary coupling condition for the pressure or an equivalent variable enforcing continuity. Two distinct techniques are investigated: (i) The instantaneous pressure is computed in a coupled fashion for the union of the LES and RANS domains and (ii) the pressure is completely decoupled and mass conservation across the interface is ensured by an adjustment of the velocities on both sides. The performance of the different methods is scrutinized for turbulent channel flow and the flow over periodic hills. It was found that the convective condition with decoupled pressure fields and an explicit mass flux correction was the most robust technique delivering results of equal or increased quality in comparison to other combinations considered.

1 Introduction

The goal of hybrid RANS-LES methods is to reduce computational cost compared to pure LES while still providing data in regions of primary interest with more information content and higher accuracy than a RANS calculation can deliver. One such approach aims for embedded LES by decomposing the entire domain into clearly identifiable regions for RANS and LES. During the simulation, the connection between these distinct zones is established at pre-defined interfaces via explicit coupling of the dependent variables. The benefit of such segregated modeling is that all turbulence closures can be computed in their regime of validity without any artificial intermediate region where neither RANS nor traditional LES modeling assumptions are likely to hold. Therefore, the turbulence closures suited best for a given purpose and complexity of the flow can be chosen for each of the sub-domains without considering their compatibility and without fear of inconsistencies in their use. The price to pay is the construction of appropriate coupling conditions at the LES-RANS interface. These need to be able to account for the sudden change in turbulence modeling and for the physical nature of the flow at the interface if a contamination of the results is to be avoided.

For LES-to-RANS type boundaries in flows with stationary statistics, the RANS zone can and should only provide mean values, whereas the LES delivers a time-dependent solution. Therefore, the coupling conditions need to allow for mean flow information to propagate upstream and for fluctuations to leave the LES domain without reflections. In the following we will constrain ourselves to a configuration with a single interface between LES and a downstream RANS zone. This setup is very instructive as an intermediate step towards wall-modeling for LES, but it is also of practical interest in its own right. One illustrative example is the flow inside a swirl-stabilized model combustor. For such a flow, the geometry far downstream of the region of primary interest has a strong upstream influence. As a consequence, a domain length focused on the region of interest with standard outflow conditions cannot be applied (Pierce & Moin, 1998). An attractive alternative to full LES or the development of more complex boundary conditions is the lengthening of the domain by adding a RANS zone and hence including the downstream effects (von Terzi *et al.*, 2005).

2 Turbulence models and numerical method

The choice of the individual turbulence model is of no concern for the present investigation. Consequently, simple, cost effective, and readily available models were employed. LES regions were computed using the Smagorinsky model with C_s=0.065 and 0.1 for the channel and hill flow simulations, respectively. The Spalart-Allmaras model was chosen as the RANS closure. For this model, a transport equation for a modified turbulent viscosity is solved requiring reasonable boundary values at the interface. These values are provided by solving the transport equation also in the LES domain, but using the explicitly Reynolds-averaged velocities.

The simulations were performed with the Finite Volume flow solver LESOCC2 (Hinterberger, 2004) developed at the Institute for Hydromechanics at the University of Karlsruhe. It solves the incompressible time-dependent filtered Navier-Stokes equations on body-fitted, collocated, curvilinear, block-structured grids. An explicit, low-storage, three-stage Runge-Kutta method is used for time advancement and second-order accurate central differences approximate the convection and diffusion fluxes. The transport equation for the modified turbulent viscosity of the RANS model is solved accordingly except that a first-order accurate partially implicit time integration is employed and that the convection term is discretized with the second-order accurate monotonic HLPA scheme.

3 Velocity coupling

Quéméré & Sagaut (2002) solved compressible transport equations, for both RANS and LES. They coupled the mean flow directly and applied a strategy they called *enrichment* to allow for unsteady fluctuations to leave the LES domain. This technique scales fluctuations from inside the LES domain and adds these to mean values obtained from the RANS domain. The so-formed total flow quantity is then copied to ghost cells at the LES domain boundary, thus mimicking an unsteady flow field on the RANS-side of the interface. Quéméré & Sagaut (2002) tested this method successfully, for both a downstream RANS zone and a zone between LES and a wall. Enrichment is a simple and easily implemented technique relying on the data exchange required anyway for multi-block domain decompositions frequently used for parallelization. However, a calibration constant C_E is needed to determine the amount of scaling of the fluctuations. There is some sensitivity of this empirically determined constant to the grid stretching at the interface and the numerical method employed and it turned out that its value must be close to but in most cases smaller than one. For other values, the method caused reflections or the solution diverged. A possible explanation for these shortcomings is given below and is illustrated in Section 5. Two cases are presented. They are denoted as E2 and E3, employing constants of $C_E = 0.1$ and 0.98, respectively.

A second, more general, and parameter-free method (von Terzi *et al.*, 2006) is assessed as well. As for enrichment, the explicitly Reynolds-averaged variable at the LES outflow is linked directly to the RANS inflow boundary, but fluctuations are convected out of the LES domain according to a one-dimensional, linear convection equation:

$$\frac{\partial \phi}{\partial t} + U_n \frac{\partial \phi}{\partial n} = 0 \tag{1}$$

where n is the direction normal to the interface, $U_n = \langle \bar{u}_n \rangle$ the averaged velocity in the n-direction, and ϕ the resolved fluctuations of the quantity to be coupled. Here, only the resolved velocities are coupled this way, hence $\phi = \bar{u}_i' = \bar{u}_i - \langle \bar{u}_i \rangle$ with the overbar representing the filter implied by LES and the brackets standing for the Reynolds average which is explicitly applied in any homogeneous spatial direction of the interface plane and in time. Using (1) for the fluctuations can be justified if the downstream transport of fluctuations across the interface is dominated by convection and if

$$U_n > 0 \text{ and } U_n >> \left|\bar{u}_n'\right| \tag{2}$$

In addition, laminar and modeled turbulent diffusion across the interface are neglected – a fair assumption for turbulent flows and adequately resolved LES.

The coupling condition of (1) is implemented in its discrete form using a first-order upwind difference in the n-direction (index j along a grid line normal to the interface) and a so-called θ-scheme (Tannehill *et al.*, 1997) with $0 \le \theta \le 1$ in time ($t = m\,\Delta t$):

$$\phi_j^{m+1} = C_1 \phi_j^m + C_2 \phi_{j-1}^m + C_3 \phi_{j-1}^{m+1} \tag{3}$$

$$C_0 = 1 + \theta\,\widetilde{U}_n \quad ; \quad C_1 = \left(1 - (1-\theta)\widetilde{U}_n\right)/C_0$$

$$C_2 = \left((1-\theta)\widetilde{U}_n\right)/C_0 \quad ; \quad C_3 = \theta\,\widetilde{U}_n / C_0$$

where, for a Finite Volume method, the interface is located at the face between the cells with index j (RANS-side) and j-1 (LES-side). For $\theta = 0.5$, as chosen for all simulations presented here, this results in the implicit second-order accurate trapezoid rule. The parameter

$$\widetilde{U}_n = U_n \Delta t / \Delta n \tag{4}$$

is the Courant-Friedrichs-Lewy (CFL) number for the convective problem. The resulting coupling conditions are then

$$U_{j-1}^{m+1} = \left\langle \overline{u}_{j-1}^{m+1} \right\rangle \tag{5}$$

for the streamwise velocity U at the inflow boundary of the RANS calculation and

$$\overline{u}_{j}^{m+1} = U_{j}^{m+1} + \overline{u}_{j}^{\prime m+1} \tag{6}$$

for the resolved streamwise velocity $\bar{u}$ at the LES outflow boundary, with $\bar{u}'$ obtained from (3). In addition, a lower bound for $\tilde{U}_n$ of 10^{-14} is enforced to ensure $U_n>0$. All other velocity components are computed accordingly. A simulation performed with the convective coupling in the form discussed above is named case C4 in order to keep the notation of von Terzi *et al.* (2006).

Setting $C_1 = C_2 = 0$ and $C_3 = C_E$ in (3), recovers the *ad hoc* formula for enrichment. Only for $U_n \rightarrow \infty$ and an implicit Euler discretization ($\theta = 1$) is it possible to derive the enrichment formula as given by Quéméré & Sagaut (2002) from (1) resulting in $C_E = 1$. Nevertheless, considering enrichment as an approximation to the discrete convective condition (3) can serve as a model to explain the difficulties with C_E described above. A single value of C_E for the simulation is then equivalent to using the same $\tilde{U}_n$ for each cell of the interface which might be a problem for configurations where $\langle \bar{u}_n \rangle$ varies strongly, e.g. for interfaces perpendicular to walls as considered in Sections 5 and 6. Negative values of the enrichment constant change the direction of the convection velocity U_n and therefore violate (2), whereas values larger than unity imply a convection velocity larger than infinity and are clearly unphysical. For $0 < C_E < 1$, enrichment lacks some terms of (3) that might cause the observed reflections. The importance of the missing terms increases with smaller values of C_E. The reflections are then likely to be larger as well if this explanation is correct. That this is indeed the case is shown in Section 5.

4 Pressure coupling

For incompressible flows, the pressure variable is governed by a Poisson-type equation whose violation has immediate consequences to mass conservation. A convective coupling as for the velocity is ill-suited for such an elliptic equation. Instead, two distinct ways of treating this variable were proposed by von Terzi *et al.* (2006): The first possibility is to solve the instantaneous pressure globally in the union of the LES and the RANS domains enforcing instant mass conservation in the complete fluid domain. The second approach is to decouple the pressure fields of the LES and RANS domains completely. In this case, both the velocity and pressure fields are discontinuous at the interface and mass conservation across this boundary is not guaranteed. Even minute mass flux deviations at each time step across the interface hamper the convergence of the Poisson solver and their accumulation may lead to a deterioration of the quality of the solution (von Terzi & Fröhlich, 2007). As a remedy, a correction can be applied to the velocities on both sides of the interface such that a desired mass flux is explicitly enforced.

The different choices of the pressure coupling and variations of the mass flux correction were already tested for the convective velocity coupling (von Terzi &

Fröhlich, 2007). For the present study, enrichment and the convective velocity coupling are compared using the same global pressure coupling whenever possible. Only in cases of its failure, the more robust method of decoupled pressure fields with mass flux correction was considered. For these cases, the velocity in the ghost cells of both sides of the interface was corrected in the following way:

First, the actual mass fluxes at the interface due to the uncorrected velocities u_i^* are computed. For the LES boundary cells, $\dot{m}_{LES}$ represents the mass flux leaving the LES domain and, for the RANS boundary cells, $\dot{m}_{RANS}$ is the mass flux entering the RANS domain. The desired mass flux at the interface $\dot{m}_{iface}$ is then determined as their average:

$$\dot{m}_{iface} = 1/2\left(\dot{m}_{LES} + \left|\dot{m}_{RANS}\right|\right) \tag{7}$$

All velocity components at ghost cells on the same side of the interface can then be scaled with the same factor

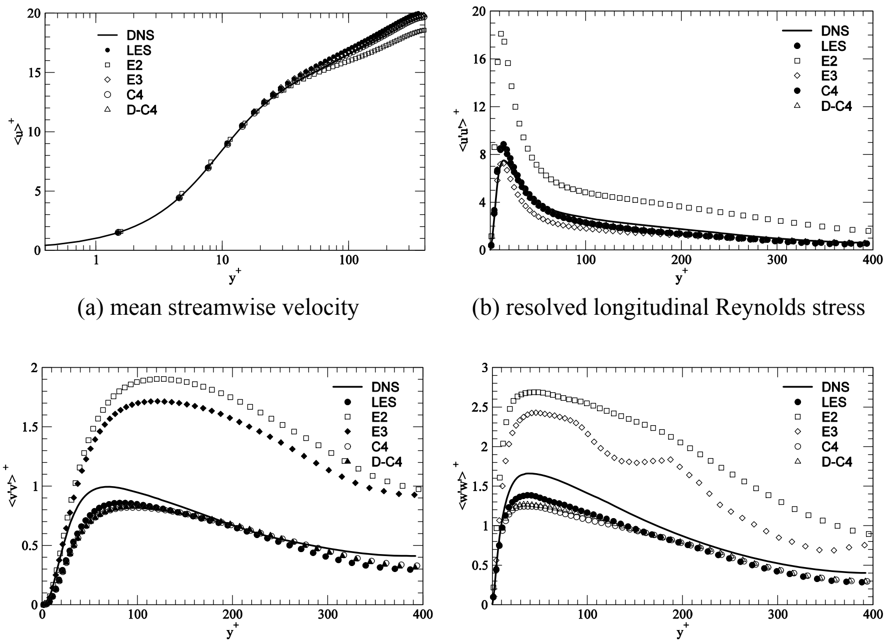
$$u_i = f_m\, u_i^* \text{ with } f_m = \frac{\dot{m}_{iface}}{\left|\dot{m}_{side}\right|} \tag{8}$$

where $\dot{m}_{side}$ is taken as $\dot{m}_{LES}$ and $\dot{m}_{RANS}$ for the ghost cells of the LES and RANS domains, respectively. The simulations using the decoupled pressure fields with this correction are marked with the prefix “D-“, i.e. cases D-C4 and D-E3.

5 Turbulent channel flow

The fully developed turbulent flow in a plane channel of infinite width is a sensitive test case for the velocity coupling conditions considered here. The reason for this is that any adverse effects due to the interfacing of LES and RANS can be immediately detected in form of streamwise variations of statistics or reflections of instantaneous quantities (von Terzi *et al.*, 2006). The specific setup is chosen to allow for comparison with Direct Numerical Simulation (DNS) data from Moser *et al.* (1999). The Reynolds number based on the friction velocity and channel half-width is Re_τ=395 and based on bulk velocity Re_b=7000. The domain is divided into three parts: the inflow generator, the principal three-dimensional LES zone and the two-dimensional RANS zone. All quantities are made dimensionless using the channel half-height δ and the bulk velocity U_b at the inlet of the principal LES zone. The inflow generator is a stand-alone LES with periodic boundary conditions in the streamwise direction and a mass flux enforced by volume forces. It provides planes of instantaneous velocities for the inflow of the principal LES zone. For each of the LES zones, the domain size is 2π x 2 x π in the streamwise (x), wall-normal (y), and spanwise (z) directions, respectively. Grid stretching is employed only in the wall-normal direction. Both domains are discretized using 80 x 100 x 80 cells resulting in a near-wall scaling of y_1^+=1.45, Δx^+=32, and Δz^+=16. The RANS domain extends over a length of 4π on a stretched grid in the streamwise direction. The same wall-normal grid as for the

LES zones is utilized with one cell in the spanwise direction. The time step was $\Delta t=0.01$ and statistics were sampled over $t=350\ \delta/U_b$ starting after steady statistics were obtained.



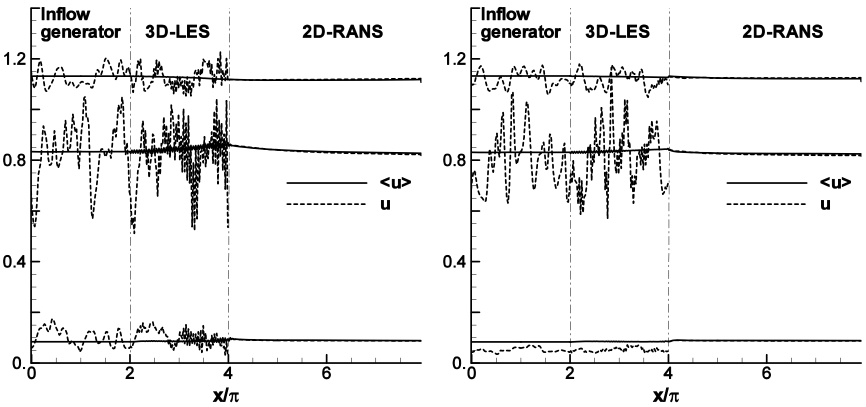
(a) mean streamwise velocity (b) resolved longitudinal Reynolds stress

(c) resolved wall-normal Reynolds stress (d) resolved lateral Reynolds stress

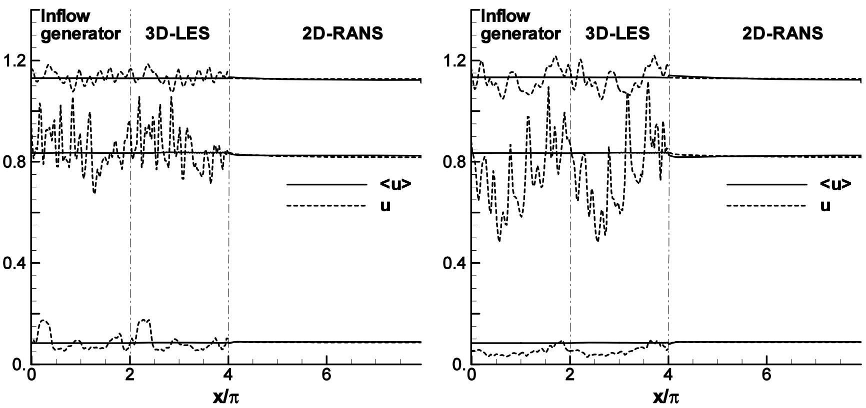
Figure 1 Turbulent channel flow: Comparison with DNS reference data of Moser *et al.* (1999) in near-wall scaling; profiles for cases E2, E3, C4, and D-C4 were taken at the grid line next to the interface, LES denotes data from the inflow generator.

Figure 1 shows the mean streamwise velocity and resolved normal Reynolds stresses in near-wall scaling for the hybrid simulations, pure LES on the same grid, and the DNS reference data. For the hybrid simulations, the profiles were taken from the grid line adjacent to the LES-RANS interface. The pure LES agrees fairly well with the DNS data with deviations in an acceptable range for the present purpose. The cases with a convective velocity coupling (C4 and D-C4) yield excellent agreement with the pure LES irrespective of the type of pressure coupling. For enrichment, the mean velocity is directly coupled and it is in good agreement with the pure LES data. However, the fluctuations are “convected” by copying a scaled value. This results in a reduced magnitude of the resolved streamwise Reynolds stress component and an increase in the other two resolved normal stress components. The strength of these deviations increases with lower values of C_E as was predicted in Section 3.

The impact of the different treatments of fluctuations at the interface on the whole flow field can be seen in Figure 2. There, the downstream development of instantaneous and mean streamwise velocity is presented at selected wall-normal locations. For the cases with convective velocity coupling, the inflow generator produces instantaneous velocities that are convected into the principal LES zone. The mean values are continuous across the LES-RANS interface and the fluctuations are successfully removed at this interface without any visible reflections. Almost the same holds for enrichment with C_E close to unity (case E3). Very weak reflections are observed at wall-normal locations close to the maximum of $<\bar{u}'\bar{u}'>^+$. However, reducing C_E to 0.1, i.e. assuming the convection velocity to be of the order of the bulk velocity (U_n = 0.8725), results in strong reflections at the interface leading to visible deviations in the mean velocity. Only case E3 will therefore be considered for further testing.



(a) enrichment with C_E=0.1 (case E2) (b) enrichment with C_E=0.98 (case E3)



(c) convective (case C4) (d) convective with decoupled pressure (case D-C4)

Figure 2 Instantaneous and mean streamwise velocities for turbulent channel flow using different velocity coupling techniques; data shown at different wall-normal locations from top to bottom: center of channel, y=0.1 (y^+=40), and y=0.0037 (y^+=1.45).

6 Periodic hill flow

Depending on the location of the interface, the flow over periodic hills can be a very discriminating test case for the downstream coupling of LES and RANS (von Terzi & Fröhlich, 2007). The configuration employed here follows Mellen *et al.* (2000), Fröhlich *et al.* (2005). The Reynolds number based on the hill height h and the bulk velocity over the crest is Re_b=10595. The distance from hill to hill is 9h, the domain height 3.036h, and the width 4.5h. Again, the simulation is divided into three distinct zones (Figure 3) with the first zone providing reference and inflow data. This zone is computed with LES using wall functions and periodic boundary conditions in the downstream direction. 200 x 64 x 92 cells are used in the downstream, wall-normal and lateral directions, respectively. LES is also performed in the second zone using the same resolution as in Zone 1. At a pre-defined location, the simulation switches from LES to RANS. The third (RANS) zone uses a two-dimensional grid and Neumann boundary conditions at the outflow. Two locations for the LES-RANS interface are considered as is illustrated in Figure 3: (i) on the crest of the hill and (ii) before the crest of the hill. 100000 time steps were computed with a variable Δt resulting in a total simulation time of roughly 390 h/U_b for case D-C4 and all cases with the interface on top of the hill, whereas only 226 h/U_b was reached for cases C4, E3, and D-E3 if the interface was placed upstream of the crest of the hill.

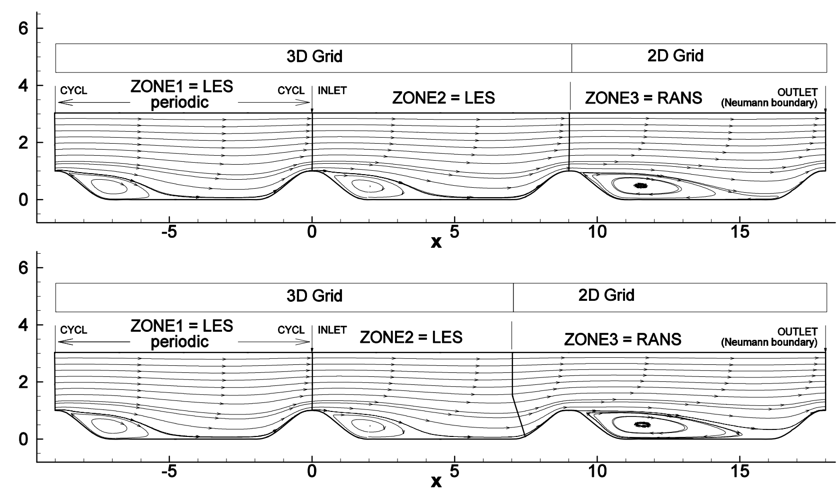


Figure 3 Setup and mean streamlines for periodic hill flow: enrichment case E3 with interface at the crest of the hill (top) and convective case D-C4 with interface at x ≈ 7 (bottom).

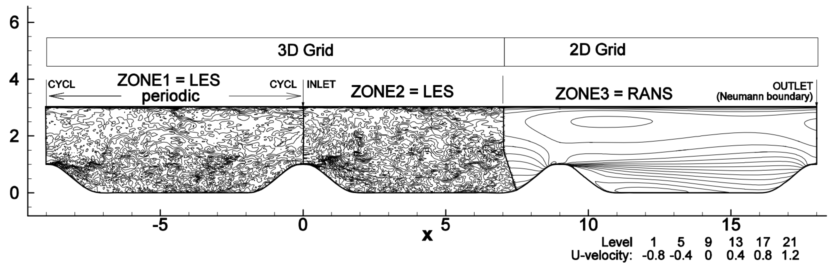
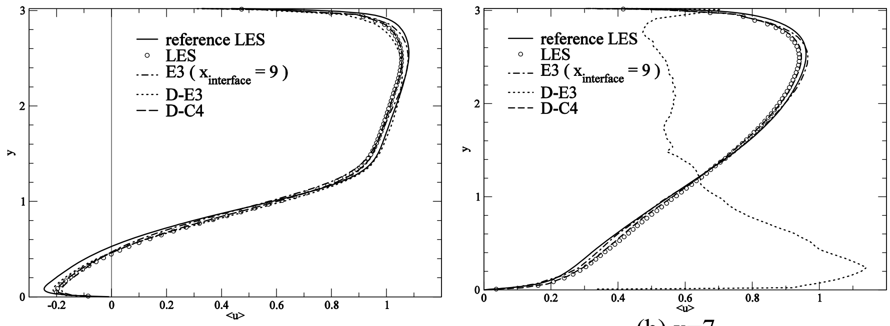


Figure 4 Periodic hill flow: Contours of instantaneous streamwise velocity for convective case D-C4 with interface at x ≈ 7.



(a) x=2 (b) x=7

Figure 5 Wall-normal profiles of mean streamwise velocity for the flow over periodic hills; reference LES data from Breuer & Jaffrézic (2005); LES denotes data from inflow generator; interface location at hill crest for case E3 and at x ≈ 7 for cases D-C4 and D-E3.

The top plot in Figure 3 shows mean streamlines for a simulation using enrichment with C_E=0.98 and global pressure coupling (case E3). The interface is located at the crest of the hill (x=9). Similar to the turbulent channel flow, this setup is uncritical and all methods tested performed well. For the bottom plot in Figure 3, the interface is moved upstream. The simulation shown was performed with the convective velocity coupling, decoupled pressure fields and the mass flux correction described in Section 4 (case D-C4). Figure 4 shows the instantaneous streamwise velocity for the same simulation. Like for the channel flow, unsteady flow structures of the inflow generator are passed on to the principle LES domain and travel downstream. At the interface to the RANS calculation, the fluctuations leave the domain without reflections, whereas the mean value is continuous (cf. Figure 3, bottom). However, using the global pressure coupling (case C4) or enrichment with any kind of pressure coupling (cases E3 or D-E3) yielded less successful results. This is demonstrated in Figure 5 for the mean streamwise velocity profiles at two locations. At x=2 (inside the region of separated flow), case D-C4 follows the LES data on the same grid quite closely, whereas the other cases exhibit only minor deviations within the accuracy of the simulation. On the other hand, at x=7, for cases with the LES-RANS interface in close proximity, only case D-C4 yields excellent results. The other cases considered here (only D-E3 shown) produce very strong reflections at the interface that lead to instantaneous reverse flow and a vastly different mean flow.

7 Conclusions

Enrichment and a convective velocity coupling combined with suitable pressure coupling techniques were scrutinized for turbulent channel flow and the flow over periodic hills. It was found that enrichment with constants C_E close to unity is a viable method for some flows. The deficits of the method, in particular for other values of C_E, were explained by analogy to the convective velocity coupling. The latter method is more general, delivers results of equal or better quality and does not require any calibration constants. For the flow over periodic hills with the LES-RANS interface upstream of the crest of the hill, only the convective velocity coupling with decoupled pressure fields and a mass flux correction at the interface was able to deliver adequate results.

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