Assessment of LES techniques for mitigating the Grey Area in DDES models

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Abstract
The slow RANS-LES transition is a well-known shortcoming in hybrid turbulence models such as Delayed-Detached Eddy Simulation (DDES). The present work assesses the feasibility of 2D sensitive LES models for naturally triggering turbulence, rather than using the specifically designed techniques available in the literature. This research has been carried out with OpenFOAM, which has been used for simulating the flow in a Backward-Facing Step configuration. The results have been compared with a DNS data set, showing the good mitigation capabilities of such LES techniques. Nevertheless, other cases should be studied before extracting any relevant conclusion.

Introduction
Accurate numerical simulations are essential for understanding the complex flow physics present in many aeronautical applications. RANS models are commonly used in the industry, as they are cost-effective, but their limitations for predicting complex flow behaviours and providing unsteady data are also well-known. Moreover, the routine use of accurate numerical methodologies such as Large Eddy Simulation (LES) require heavy computational cost, so their applications are not yet feasible. In this regard, Delayed-Detached Eddy Simulation (DDES) is intended to circumvent the massive costs of pure LES simulations, modelling the boundary layer using RANS and simulating the unsteady flow behaviour with LES at the core. This hybrid turbulence model is widely used due to its user-friendly non-zonal approach and its proved success in several applications. Especially in those situations where RANS applications are unreliable. Apart from that, hybrid turbulence models (in contrast to RANS) can provide high quality transient data, which is completely necessary for simulating complex coupled physics, such as Fluid-Structure Interaction (FSI) and Computational Aeroacoustics (CAA). It is therefore not surprising that during the last decade, these methods have been gaining importance in the aeronautical industry. However, some of their well-known weaknesses are still present. In particular, the slow transition from RANS to LES leads to unphysical results, delaying the flow instabilities in complex zones such as free shear layers. The zone where this issue takes place is named Grey Area (GA). In the literature, there are two main strategies for leading this shortcoming. One of them consists on using artificial oscillations in specific areas (zonal approach), whereas the other is based on reducing the subgrid-scale viscosity,

\[ \nu_{sgs} = (C_m\Delta) D_{sgs}(\bar{u}), \]

\( \nu_{sgs} \) in LES 2D flow regions. The second approach is preferable as it is aligned with the initial non-zonal DES philosophy. This reduction could be forced by any of the terms present in Eq. 1. The idea of attributing kinematic sensitivity to the Subgrid-Length Scale (SLS) coefficient, \( \Delta \), was initially explored by Mockett et al. (\( \Delta_{\omega} \)) and Shur et al. (\( \Delta_{SLA} \)). Later we proposed another approach, which was initially developed for LES \( \Delta_{iso} \). Surprisingly, even though \( \Delta_{iso} \) was initially designed for LES applications, first studies show how its performance mitigating the GA in DDES was
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Figure 1: Schematic figure of the Backward Facing Step problem, $ER = H/(H - h) = 2$, and details about its geometry and grid spacing (size of zones and concentration factors; arrows indicate the grid refinement direction). Not to scale.

rather promising. It is important noting here that, in contrast to the other specifically designed techniques for mitigating the GA shortcoming, $\Delta_{lsq}$ is completely based on a physical and mathematical basis.

The significant influence of the differential operator, $D_{sgs}(\bar{u})$, into the GA mitigation was also reported in the literature. Some authors such as Fuchs et al.\(^2\) and Probst et al.\(^7\) investigated the impact of using the $\sigma - LES$ model, instead of Smagorinsky, due to its ability for switching off in 2D flow regions. Taking into account that unsteady 2D flows can not be considered as turbulent, the idea of deactivating the model in such regions look reasonable. In fact, the $\Delta_{SLA}$ presented by Shur et al.\(^8\) was also based on the same approach (Eq. 2), as the $\Delta$ turned zero in 2D flow regions. Therefore, both strategies strengthen the importance of deactivating the turbulence model in 2D flow areas.

\[ \nu_{sgs} = (C_m \Delta_{SLA})^2 D_{sgs}(\bar{u}) = (C_m \tilde{\Delta})^2 (F_{KH}(\langle VT M \rangle)^2 D_{sgs}(\bar{u})) = (C_m \tilde{\Delta})^2 D_{sgs}^{2D}(\bar{u}). \] (2)

In this paper, the mitigation capabilities of both strategies, $\Delta$ and $D_{sgs}(\bar{u})$, are analysed. The selected configuration case for assessing these methodologies is an incompressible Backward-Facing Step (BFS). The fact that the flow separation is purely induced by geometry, makes this case suitable case for studying the GA numerical issue.

Case Description

Backward-Facing Step represents a canonical configuration to study wall-bounded fluids subjected to sudden expansions (see figure 1). The flow is massively separated at the step-edge, but downstream reattached due to the geometry. The abrupt separation leads to a shear layer, which becomes a source of the well-known Kelvin-Helmholtz instabilities (KH) at high enough $Re$ values. These instabilities are fed, paired and elongated along the shear layer, affecting the flow behaviour until they impinge at the lower wall. These instabilities are not always well-captured for Hybrid RANS-LES turbulence models due to its slow RANS to LES transition. The fact that the flow separation is purely induced by geometry, makes the BFS a suitable case for studying such numerical issue.

The selected dimensions are $24h \times 2h \times 2h$ in the stream-wise, cross-stream and span-wise direction, respectively. The sudden expansion with an expansion ratio, $ER = H/(H - h)$, equal to 2 is located at $L_u = 4h$ from the inflow. The domain length downstream of the step is $L_d = 20h$. The origin of coordinates is placed at the sharp edge. Regarding the mesh, three different refinement levels at the free shear layer (stream-wise direction downstream the step-edge) have been considered for evaluating the mesh resilience capabilities of the studied strategies. The length of the first node after the step-edge in the stream-wise direction is 8, 16 and 32 times $y^+$ (inflow conditions). All meshes have 11800 cells per xy-plane and 60 planes in the periodic direction. Concerning the boundary conditions, the inflow is fed with a steady (but turbulent) channel flow profile at $Re_\tau = 395$, which has obtained from a previous RANS simulation. The span-wise and outflow boundary conditions are defined as periodic and convective, respectively. Walls are considered no-slip.
**Mathematical Model**

All simulations carried out in this study have been run using *OpenFOAM - v1706*. The DDES turbulence model presented by Spalart et al.\(^9\) has been used, including the $\Psi$ term specially designed to override the unintended low-Re terms. The Hybrid convection scheme presented by Travin et al.\(^11\) for hybrid RANS/LES calculations is used in this simulation. For the temporal discretisation, a 2ⁿ implicit backward scheme is considered with *Courant* values below 0.8. The velocity-pressure system is coupled using the well-known *PISO* algorithm.

**Definition of the $\Delta$’s**

A brief introduction about the subgrid-length scales assessed in this paper is presented. First, the volume cubic root was initially presented by Deadorff,\(^1\)

$$\Delta_{vol} = (\Delta x \Delta y \Delta z)^{1/3}, \quad (3)$$

which by far is the most widely used for LES applications. Later on, the maximum length scale,

$$\Delta_{max} = \max (\Delta x, \Delta y, \Delta z) \quad (4)$$

was introduced in the first DES version,\(^10\) as a good candidate for dividing the RANS and LES regions. However, Mockett et al.\(^4\) and Shur et al.\(^8\) observed as both definitions, $\Delta_{vol}$ and $\Delta_{max}$, were inextricably linked to unintended length scale changes due to mesh variations, as neither one considers the kinematic fluid behaviour. This directly leads to a poor mesh resilience for anisotropic meshes. In this context, a kinematic sensitive approach resistant to mesh length scale changes due to mesh variations, as neither one considers the kinematic fluid behaviour. This directly leads to a poor mesh resilience for anisotropic meshes. This context, a kinematic sensitive approach resistant to mesh anisotropies was proposed by Mockett et al.\(^3\),

$$\tilde{\Delta}_w = \frac{1}{\sqrt{3}} \max_{n=1,...,8} |I_n - I_{ref}|,$$  \( (5) \)

defining the importance of the maximum meaningful scale at each LES control volume. This method was improved by Shur et al.\(^8\) for DDES/IDDES applications, where a rapid transition from RANS to LES is required to avoid unphysical instability delays,

$$\Delta_{SLA} = \tilde{\Delta}_w F_{KH}(VTM). \quad (6)$$

Where $l = \omega ||\omega|| \times r_n$, $r_n$ (n=1,...,8 for hexahedral cell) are the locations of the cell vertices and $F_{KH}$ is a blending function which depends on the average *Vortex Tilting Measure* coefficient defined in Eq. 7.

$$VTM = \frac{\langle S \cdot \omega \rangle \times \omega}{\omega^2 \sqrt{-Q_S}} \quad (7)$$

Where $\hat{S}$ is the traceless part of the rate-of-strain tensor, $S = 1/2 (\nabla \bar{u} + \nabla \bar{u}^T)$, i.e. $\hat{S} = S - 1/3tr(S)I$. Note that for incompressible flows $tr(S) = \nabla \cdot \bar{u} = 0$, therefore, $\hat{S} = S$. Finally, $Q_A$ refers to the second invariant of a second-order tensor A. Although successful results have been obtained for a broad spectrum of fluid behaviours,\(^3,4,8\) a lack of physical meaning can be attributed to $\tilde{\Delta}_w$. In this regard, Trias et al.\(^12\) suggested a new subgrid length scale only based on the velocity gradient, $\Delta_{tg}$. This subgrid length scale, which is derived from physical LES well-established assumptions, is not only resistant to grid anisotropies but also computationally inexpensive and adapted for any sort of grid, structured and unstructured ones.

$$\Delta_{tg} = \sqrt{\frac{JG^T G : JG^T G}{G^T G : G^T G}} J = \left[ \begin{array}{ccc} J_{11} & J_{12}^T & J_{13}^T \\ J_{12} & J_{22} & J_{23}^T \\ J_{13} & J_{23} & J_{33} \end{array} \right], J_{ij} = \frac{1}{\sum_{j=1}^{3} \|G_{ij}\|} \quad (8)$$

Where $J$ is the Jacobian, which collapses to $J = diag(\Delta x, \Delta y, \Delta z)$ in a Cartesian structured and non-uniform mesh. $G_{ij}$ refers to the components of the gradient operator, $G$, in the $l$ direction. It is important to note that the gradient tensor, $G$, is actually being computed in any LES and DES code. The $\Delta_{tg}$ approach was tested in LES simulations (incompressible flow) using different kind of anisotropic meshes, showing good mesh resilience in all cases.

**Results**

For the sake of clarity, the effect of $\Delta$ and $D_{sgs}(\bar{u})$ has been studied separately. The former is focused on the influence of $\Delta$, keeping the LES turbulence model constant ($SMG$). The fact that $\Delta$ does not only influence the $\nu_{sgs}$, but also limits the RANS/LES region is a crucial aspect for understanding the observed results. The latter mainly affects the $\nu_{sgs}$ value, but also has a significant impact improving the $rms$ values at the GA (especially, those differential operators sensitive to 2D flows).
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The influence of the aspect ratio, $\Delta x_1/\Delta x_2$, at the first cell downstream of the step edge is first discussed using the results shown in Fig. 2. For this purpose, three slightly different meshes have been used (see section 2). The highest aspect ratio (right) presents some non-physical oscillations at $x_1/h = 0$. This is not the case for the other two figures (left, centre), where the aspect ratio is considerably smaller. Apart from that, the performance of the SLS in different meshes can also be appreciated. A general good mesh resilience is observed for $\Delta \omega$, and for $\Delta_{SLS}$, whereas $\Delta_{lsq}$ presents a strong mesh dependency. It can be justified, taking into account that $\Delta_{lsq}$ strongly depends on the stream-wise cell length in 2D flow configurations. This is not the case for $\Delta_{SLS}$ and $\Delta_{lsq}$, as the former is deactivated in 2D flow areas and the latter mainly depends on the normal cell due to the flow kinematics in such region. Taking into account the results observed in Fig. 2, from now on the rest of results have been obtained using the mesh with $\Delta x_1/\Delta x_2 = 16$ (middle). The evolution of the mean flow and the $rms$ in the stream-wise direction at different positions is shown in figure 3. In this case, we can observe how the mean flow is almost non-affected, whereas the $rms$ present only significative differences at the free shear layer zone, where the GA shortcoming takes place (Fig. 2).

The effect of the GA into the growth of instabilities at the shear layer is also analysed using the same approach described by Pont-Vílchez et al. A scheme view of this phenomenon is presented in figure 4 (left). The characteristic length of the instabilities in the stream-wise direction, $\delta_1$, is calculated using a set of 2-point correlations of $u'_1$ along the stream-wise direction downstream of the step-edge (Fig. 4). Unfortunately, this technique cannot be applied for assessing the size of instabilities in the normal direction, $\delta_2$, as the flow behaves laminarly in some parts along the normal direction. For this reason, another approach based on mean quantities has been used,\(^5,13\)

\[ \Delta \delta_2 = \Delta U_1/(\partial (\langle u_1 \rangle / \partial x_2)_{\max}). \] (9)

Even though the $rms$ profiles present a strong dependence on the SLS (Fig. 2) along the shear layer, this is not so significant in the $\Delta \delta_1$ distribution (Fig.4). In particular, $\Delta_{lsq}$, together with $\Delta_{SLS}$, show the best alignment at $x_1 \in [0,0.7h]$. However, the strength of correlation with DNS data is notably reduced further downstream, leading to a distinct departure of the slope gradient from the reference data, which is mainly attributed to the mesh coarsening in this region. Regarding $\Delta \delta_2$, it seems to be quite sensitive to the SLS (such as $rms$ profiles), presenting strong differences in values and slopes (Fig. 5). The fact that we are using Eq.9, instead of a 2-point correlation along the normal direction, plays an important role as $\partial (\langle u_1 \rangle / \partial x_2)_{\max}$ is highly influenced by the $rms$. This is clearly observed in figure 5 (right) where the diffusion introduced by $\Delta_{SLS}$ and $\Delta_{lsq}$ may be permitted to grow to excessive levels, preventing the KH instabilities from properly developing along the shear layer.
Figure 3: Mean velocity (top), $\langle u_1 \rangle$, and resolved Reynolds stresses (bottom), $u_{rms}^1$, along the recirculation region downstream the step edge. Reference solid line has been obtained from Pont-Vílchez et al.\textsuperscript{5}

Figure 4: Schematic view of the KH vortices in a shear layer (left) and estimation of the KH rate of growth in the streamwise direction downstream of the step-edge, $\Delta \delta_1$ (right). Different SLS definitions have been used. Reference solid line has been obtained from Pont-Vílchez et al.\textsuperscript{5}
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Figure 5: Schematic view of the KH vortices in a shear layer (left) and estimation of the KH rate of growth in the streamwise direction downstream of the step-edge, $\Delta \delta_1$ (right). Different SLS definitions have been used. Reference solid line has been obtained from Pont-Vilchez et al.\textsuperscript{3}

Differential operator, $D_{sgs}$ ($\bar{u}$)

A set of simulations using different operators is presented, including $\Delta_{SLA,SMG}$, $\bar{\Delta}_u$, $\sigma - LES$; $\bar{\Delta}_u$, $S3QR$ and $\Delta_{lsq,SMG}$, $S3QR$\textsuperscript{6}. In this case all turbulence models are able to be deactivated in free shear layer 2D flow domains, either by $\Delta_{SLA}$ or $D_{sgs}^{DDES}$ ($\bar{u}$). Different $rms$ profiles along the recirculation region are shown in figure 6, as well as the $rms$ distribution along the shear layer after the step-edge. Even though a similar positive and linear trend is observed in all cases, the $\Delta_{lsq}$ in combination with the $S3QR$ provides significantly better results than the other strategies. However, the comparison between the $rms$ distribution along the stream-wise direction (bottom) with Fig. 2 (middle) indicates that the $S3QR$ turbulence models has a little, if any, contribution to the final result. This is mainly attributed to the predominance of the $\Delta$, which contributes to the definition of the RANS and LES regions. This is not the case for the differential operator, which only affects the $\nu_{sgs}$ value in the LES area. Regarding $\bar{\Delta}_u$, both $S3QR$ and $\sigma - LES$ improve the mesh resilience capabilities of the SLS (Fig. 2), which is directly observed in figure 6 (bottom). These results are really similar to those provided by $\Delta_{SLA,SMG}$, supporting the observations made in section 1. Indeed, the results observed in this section are in good agreement with the studies carried out by Fuchs et al.\textsuperscript{2} and Probst et al.,\textsuperscript{7} regarding the importance of using $D_{sgs}$ ($\bar{u}$) sensitive to 2D flows. The growth of the shear layer instabilities along the stream-wise and normal directions is also studied. The former is not shown in this paper, as all simulations exhibit trends similar to those presented in figure 4 (right). The latter is shown in figure 7. In this case, we can observe again the benefits provided by $\sigma - LES$ and $S3QR$ in comparison to $SMG$.

Conclusions

This work shows how both techniques, $\Delta_{lsq}$ and $D_{sgs}^{DDES}$ ($\bar{u}$), which were initially developed in a LES context, are capable of mitigating the GA numerical issue. In particular, the use of $\Delta_{lsq}$ provides substantial benefits in the free shear layer area respect to the rest of SLS strategies. Moreover, the influence of those $D_{sgs}$ ($\bar{u}$) sensitive to 2D is also noticed. Especially in combination with those $\Delta$ which are too sensitive to the stream-wise meshing (such as $\bar{\Delta}_u$). Apparently, the use of such differential operators, $D_{sgs}^{DDES}$ ($\bar{u}$), clearly improves the mesh resilience capabilities of DDES in 2D LES flow regions. The fact that $\Delta$ does not only influence the $\nu_{sgs}$, but also defines the RANS/LES regions, explains the significant better results observed by $\Delta_{lsq}$ in comparison to the other strategies. Finally, the assessment of the differential operators also show the similarity between the $\Delta_{SLA}$ and those $D_{sgs}$ ($\bar{u}$) sensitive to 2D flow regions. While further work is required to investigate whether these observations hold in other flow configurations, these initial results indicate how both $\Delta_{lsq}$ and $D_{sgs}^{DDES}$ ($\bar{u}$) are promising strategies for naturally mitigating the RANS to LES numerical delay.

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Figure 6: Resolved Reynolds stresses, $u_{rms1}$, along the recirculation region downstream the step edge (top) and its evolution in the stream-wise direction (bottom). Reference solid line has been obtained from Pont-Vilchez et al.\textsuperscript{5}

Figure 7: Estimation of the KH rate of growth in the normal direction, $\Delta \delta_2$, downstream of the step-edge using different strategies sensitive to 2D flow regions. Where $U_o$ refers to the inflow bulk velocity.
References


