Embedded LES Methodology for General-Purpose CFD Solvers

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ABSTRACT
The goal of this paper is to describe the implementation of an embedded LES module into an industrial CFD solver. In this technique, the Large Eddy Simulation approach exists as a sub-domain within a broader RANS domain. The approach itself poses several challenges, both from the physical modelling point of view, as well as from the point of code organization and infrastructure. The main physics challenges are present at the interfaces between RANS and LES zones and special attention will be given to those aspects in this paper.

The main motivation behind this work is to answer the question whether such technique can be used as a general predicting tool for industrial turbulent flows. The following flows have been considered: fully developed pipe, channel flow and flow over a backward facing step. It is shown that this technique coupled with suitable solver technology is capable of delivering accurate results across different test cases. This in turn means that with increasing computer power, it can serve as a practical bridge between full RANS and full LES simulations.

INTRODUCTION
For many decades, the two main approaches of turbulence modelling, namely Reynolds Averaged Navier-Stokes (RANS) modelling and Large Eddy Simulation (LES) existed mutually exclusive. While RANS was, and still is, the work horse for industrial CFD simulations, it is clear that LES offers significant potential in situations where RANS is overly restrictive, or does not provide the required unsteady information. Examples are flows with large separation zones (where RANS models typically underestimate the amount of turbulent mixing) or flows where unsteady information is required (like in the simulation of acoustic phenomena). It is also clear that in the near future, LES will not be able to replace RANS modelling for complex industrial applications, due to the high resolution demands, especially near walls.

There is a growing recognition that RANS and LES models can be combined into formulations preserving the advantages of each one of the two concepts. This can be achieved in many different ways; the most widely used being Detached Eddy Simulation (DES) and variants of it (Spalart, 2000). DES in its original form is a "global" approach which uses a single model formulation in the entire domain. The model by itself blends between RANS and LES formulations based on the solution and the spacing of the numerical grid. Due to the rather different requirements for the underlying numerical schemes for RANS and LES, an additional blending is required for the discretization of the convective terms. This approach is very successful for flows, where the flow physics can be divided into mostly attached regions, and regions with strong separation connected by a zone of severe instabilities between them. Under such conditions there is no need for introducing unsteady fluctuations explicitly at the "interface" between the regions of different flow physics.

While such situations are frequently encountered in industrial flows, there are also applications where a tighter control over the different zones is required. In such cases, it is desirable to define a clear interface between RANS and LES regions. At these interfaces, the code will then switch both - the turbulence model and the numerical scheme - in a more defined and controlled fashion than in the case of standard DES. This leads to the formulation of zonal approaches where the user pre-specifies the desired modelling concept for the given zones, ahead of the simulation. From a code development standpoint, this requires the formulation and implementation of interface conditions which provide a physically correct transfer of information between the models involved on both sides of the interface. The current paper will deal with such an explicit interfacing of RANS and LES methods (e.g.
Quemere and Sagaut, 2002), typically known as embedded LES (ELES).

ELES REQUIREMENT
The ELES formulation has typically been developed within special-purpose codes and often only for specific types of test cases. This is a prudent approach for developing new technologies, but more generality is required when using this technique in a general-purpose industrial CFD environment. Thus when implementing ELES methods into an industrial code environment, a general embedded LES capability needs to be able to provide (at minimum) the following capabilities:

1. Ability to treat any pre-defined fluid zone as a LES zone within a global RANS domain
2. Ability to use local non-dissipative spatial discretisation scheme (e.g. central differencing) within the LES zone regardless of the global RANS scheme used elsewhere
3. Ability to apply any sub-grid LES model in conjunction with filtered Navier Stokes equations regardless of global RANS turbulence model
4. Ability to use LES wall treatment for the walls adjacent to the LES zone regardless of global RANS wall treatment.
5. Ability to generate unsteady flow fluctuations at RANS/LES interface
6. Ability to provide RANS turbulence at LES/RANS interface.

Despite the fact that the inclusion of all of the above capabilities into a single code environment presents a substantial challenge, there is no doubt that from the physical standpoint, the most interesting aspect is the treatment of the interfaces between two zones.

ELES METHODOLOGY
Obviously, there are many possible choices in the way the models are combined and interfaced, and not all can be handled by a single interface formulation. The most common conditions are inlet (RANS/LES) and outlet situations (LES/RANS) where the flow mainly (or always) enters or leaves the LES domain through the interface.

RANS/LES interface

While the formulation on the RANS/LES interface is clearly a critical element of the ELES method, it can be mostly compiled from existing techniques available in the solver. The central module is the Vortex Method (Mathey et al., 2006), currently applied to true LES inlet boundaries (e.g. velocity inlets, pressure inlets etc.). It generates turbulent structures based on information provided from a RANS model (Reynolds stresses and length scale). The infrastructure within the code is modified to allow the application of the VM at any interior interface. The RANS information is obtained from the RANS model used upstream of the interface.

LES/RANS interface

A more open question concerns the treatment of the LES/RANS interface. There are several options which will be investigated. For the sake of argument, one approach could be to run RANS turbulence transport equations in a passive mode (i.e. not coupled with the momentum equations) inside the LES domain. The model would then automatically provide RANS turbulence quantities as the flow re-enters the RANS zone downstream from the LES zone. However, RANS transport equations would then be subject to "double accounting" of turbulence, as turbulence structures as well as RANS turbulent kinetic energy, would be transported across the interface. This approach would produce excessive amounts of turbulent kinetic energy. This is mainly due to the high production rates of the RANS model inside the LES zone. In LES, the shear strain rates are on average substantially higher than in a RANS zone. This is due to the high strain rates of the small eddies. The passive mode of the RANS model will therefore result in an excessive production inside the LES zone resulting in large levels of modelled kinetic energy, which would then be convected into the RANS region via LES/RANS interface.

Approach 1: RANS frozen field

The above mentioned problems could be avoided by running a pre-cursor RANS simulation and freezing the RANS turbulence quantities in the LES zone during the ELES run. This will result in lower RANS levels and reduce some of the issues with the previous approach. Again, no treatment is applied to the velocity field at the interface (meaning unsteady velocity would be used to transport RANS turbulence back into the RANS region). It will be shown that this concept works reasonably well. However, from a theoretical standpoint, there is still some "double accounting" of turbulence as turbulence structures as well as RANS turbulent kinetic energy is transported through the interface. Potential problems with this approach are anticipated in cases where the RANS and the ELES solutions differ substantially. In the worst case, the ELES could result in a topology change and the frozen RANS solution would no longer correspond to the actual flow situation. In the current paper, the impact of this concept will be explored only for simple flow configurations.

Approach 2: SAS solution inside LES zone

"Double accounting" can be avoided all together if the underlying RANS transport equations have a mechanism that can adapt itself to any scales fed into them, via the velocity field generated inside the LES zone. One such model possessing such a feature is the Scale-Adaptive Simulation model (SAS) (Menter and Egorov, 2004). SAS models are derived based on RANS arguments using the theory of Rotta, 1972, for the formulation of the length-scale equation. Based on this concept, the SAS model features the von Karman length scale \( \ell_k \) in the scale equation. As has been demonstrated in a series of papers, the inclusion of \( \ell_k \) allows the model to adjust to locally resolved scales and produce LES-like solutions in strongly unstable flows. In the current context, the SAS model offers the advantage that it can be run in passive mode in the LES
zone, without producing excessive levels of turbulent kinetic energy (or eddy-viscosity). Downstream of the interface, the model is then used in active mode again, damping out the resolved structures and returning the solution to RANS mode. The ability of the SAS method to recognize resolved structures results in a "soft" interface condition, which produces a smooth variation from LES back to RANS.

Sub-grid scale modelling

Assuming that an eddy-viscosity, \( \nu_e \), is used both on the RANS and LES side, the momentum equations can be written as:

\[
\frac{\partial \bar{p}}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \nu + \nu_e \right) \frac{\partial \bar{u}_i}{\partial x_j}.
\]

The ELES approach could accommodate any sub-grid model, but for the sake of simplicity and since sub-grid modelling is not the main interest of this paper, we chose in this study to use WALE model of Nicoud and Ducros, 1999. Note that in the current implementation, the RANS model can also be a Reynolds Stress formulation.

Numerical methods

The computations were carried out using the general-purpose CFD software ANSYS-FLUENT. ANSYS-FLUENT employs a cell-centred finite-volume method, based on a multi-dimensional linear reconstruction scheme that permits use of computational elements (cells) with arbitrary polyhedral cell topology, including quadrilateral, hexahedral, triangular, tetrahedral, pyramidal, prismatic, and hybrid meshes. The solution gradients at cell centres, which are needed to compute convective and diffusive fluxes, are obtained by applying Green-Gauss theorem. Diffusive and convective fluxes are discretized using central differencing scheme. However, the convective fluxes outside the LES zone were calculated using a second order upwind scheme.

RESULTS

The ELES approach described above has been applied to the test cases described below: fully-developed pipe flow, fully developed channel flow and flow over backward facing step.

Fully Developed Pipe Flow

A typical scenario for RANS/LES interface is given in Figure 1, showing the mesh and domain for a pipe flow, with a RANS zone (k-\( \varepsilon \) model used) in the upstream part and a LES zone in the downstream section. For this initial test the mesh resolution is kept identical between LES and RANS zones giving a total number of cells of 112000. The Reynolds number is \( Re=5000 \). The streamwise velocity contours at various locations are shown in Figure 2. As the flow does not supply a strong instability past the interface, it is not sufficient to simply switch models and numerical formulations. In addition, it is also essential to introduce turbulent eddies at the interface in order to provide a smooth variation of time averaged flow features, like turbulent kinetic energy, wall shear stress or pressure drop. In the proposed formulation, these fluctuations are generated using an artificial vortex method, which converts the information from the RANS model into coherent turbulent eddies. This can be seen in Figure 2b where the synthesized velocity field is displayed, obtained using the VM and the incoming flow RANS velocity (shown in Figure 2a). The Vortex Method approach has proven much more efficient than simply providing random fluctuations, which have been found to die out quickly in channel flow simulations. Consequently the turbulence and flow fluctuations are maintained downstream of the RANS/LES interface, as can be seen in Figure 2c. This is at \( x=6 \) where the instantaneous velocity downstream the RANS/LES interface still maintains the physical fluctuations and compares well with fully developed results obtained using periodic boundary conditions (Figure 2d).

Fully developed channel flow, \( Re=395 \)

Fully developed channel flow, for which detailed DNS data exists, is chosen for detailed testing of the RANS/LES interface. The domain consists of the RANS zone being attached to the inlet, followed by the LES zone and again followed by another RANS zone that ends with the outflow, as shown in Figure 3. Again, the mesh resolution is kept the same between different zones. The size of the domain is shown in Figure 3. The mesh resolution is chosen to have 72 and 74 cells respectively in normal and span-wise direction while in the stream-wise direction is 161 covering all zones, resulting in an overall mesh of 857808 cells. DNS data (Moser et al., 1998) is available for this flow field, providing both mean and rms profiles. The VM was used at the RANS/LES interface to randomly perturb the fully developed mean velocity profile. This mean-velocity profile was extracted from the RANS calculations, upstream of the interface. The time-averaged profiles of the DNS and the ELES calculation are compared in Figure 4. The mean velocity profiles at \( x=1.5 \pi \) from the RANS/LES interface agree very well with DNS data as well as the theoretical wall velocity profiles. In particular, it is noteworthy that the profile is preserved so far downstream from the interface, indicating that there is self-preservation of turbulence quantities inside the LES zone downstream from the interface. This is further emphasized by the predicted velocity fluctuation in all three directions shown in Figure 5. There, the peak value of the stream-wise velocity fluctuation close to wall is reasonably accurate; however the level is under-predicted at the centre of the channel. The span-wise and wall-normal fluctuations are in good agreement both close to wall, and in the channel centre. With iso-surfaces of the q-criterion, the turbulent flow structure can be visualized, see Figure 6. In both RANS regions the turbulent structures disappear, as they are modelled there. Within the LES zone vortex stretching is clearly visible. Further on, the vortices do not decay in downstream direction.

Backward Facing Step

As a more stringent test, a backward facing step is chosen for testing of the LES/RANS interface as shown in Figure 7. In this case there are three different zones. Upstream of the step, the flow is computed in RANS mode (Reynolds Stress Model used). In the re-circulation zone, the code runs in LES mode and downstream of the
separation, the simulation reverts back to RANS. This test case was used to test two approaches presented earlier in the paper for modelling the flow at the LES/RANS interface, where the flow exits the LES zone and re-enters RANS zone.

The back step mesh is shown in Figure 7 depicting the refined mesh within the LES zone. The total mesh size is 278800 out of which 77% is concentrated within the LES region.

A first set of simulations was conducted using Approach 1 whereby the full Reynolds stress model solution of turbulence was frozen (from the pre-cursor RANS simulation) inside the LES zone to provide inflow conditions for the downstream RANS region. The velocity contours are shown in Figure 8. Figure 8a shows instantaneous velocity contours in which LES structures exist within the LES zone. The flow structures in the RANS zone downstream of the LES zone resemble classical unsteady RANS type of flow features. However, when time averaged the results show velocity contours that one would expect to see for a backward step, as can be seen when comparing the results with steady state RANS solution shown in Figure 8c. Furthermore, it is a natural consequence of using the LES technique that there should be improvements in quality of prediction within the zone where LES is employed. In this case this is visible in the improved velocity profiles in the separation zone, compared to the RSM solution. This is clearly indicated by comparing velocity profiles at various locations inside the LES zone, as shown in Figure 9. However, the main issue in this section is what happens after the LES/RANS interface. The idea being that one would not want to see a negative impact of the LES/RANS interface modelling on the quality of the predicted results further downstream. For that reason we compare velocity profiles at $x^*=0.6$ (with $x^* = (x-\tau_{reattach}) / \tau_{reattach}$) just inside the RANS zone) obtained by using ELES and full RANS simulations (no exp. profiles available past the interface). It clearly shows that RANS results are not compromised by the presence of LES/RANS interface further downstream despite partial “double accounting” that may be present in this approach.

An identical exercise was repeated using Approach 2, in which as mentioned previously, the SAS model was used to passively solve the turbulence equations in the background of the LES zone in order to provide turbulence quantities at the LES/RANS interface. The stream-wise velocity contours, as predicted by this approach, are shown in Figure 11. The contours within the LES zone exhibit the same features as with the previous approach while the contours downstream of the LES zone show more unsteadiness than before. This is normal, given the ability of SAS to be more able to naturally model unsteady flows. However, time averaged contours obtained by ELES are very similar to those obtained by running the SAS in steady state mode (pre-cursor). Given the fact that the steady-state SST-SAS model predictions in the recirculation region behind the back step are reasonably accurate, there is very little difference between steady SAS and ELES results for the velocity profiles there, as shown in Figure 12. However, more importantly the turbulence field provided by SAS at the LES/RANS interface leads to very smooth conditions, resulting in almost unaffected velocity profiles downstream of the interface. This is indicated in Figure 13 where the ELES prediction for mean velocity profile is almost identical, compared with the separate steady SAS simulation. The iso-surfaces of the q-criterion in Figure 14 and 15 shows that turbulent structures are resolved in the LES zone and that they do not decay there. Within the outflow RANS zone, the turbulence decays and reverts back to RANS. As expected the ELES using the SAS model in the background of the LES zone decays much slower than the standard RANS models.

**CONCLUSION**

Embedded LES simulations of three different flows have been conducted. Particular attention was given to testing options to represent the RANS/LES and LES/RANS interfaces. For the RANS/LES interface the standard Vortex Method approach was used. Two different approaches were considered at the LES/RANS interface: a frozen RANS turbulence field and a passive background solution of the SAS equations. The level of accuracy of all predicted cases was a very satisfactory which confirms the view that the ELES technique has matured to a point where it can serve as a bridge between the traditional RANS and the more elaborate (but still expensive) LES method.

**REFERENCES**


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Figure 1. Fully developed pipe flow. Domain and mesh at different cross sections.

Figure 2. Fully developed pipe flow. Stream wise velocity contours.

Figure 3. Fully developed 3D channel flow. \(Re_{\tau}=395\) domain and mesh

Figure 4. Fully developed channel flow. Mean velocity values inside LES zone.

Figure 5. Channel flow. Rms values inside LES zone at \(x = 1.5+1.5\pi\).

Figure 6. Channel flow. Viscosity ratio on iso-surfaces of q-criterion (500).

Figure 7. Back step. Domain and mesh distribution per zone.
a) ELES inside RSM: Instantaneous U velocity.

b) ELES inside RSM: Time-averaged U velocity.

c) RANS (RSM) all zone: U velocity.

Figure 8. Backward facing step. U velocity contours.

Figure 9. Backward facing step. Mean velocity profiles inside LES zone.

Figure 10. Backward facing step. Mean velocity profiles inside RANS (RSM) zone at $X^* = 0.6$ (just after LES zone).

Figure 11. Backward facing step. U velocity contours.

Figure 12. Backward facing step. Mean velocity profiles inside LES zone.

Figure 13. Backward facing step. Mean velocity profiles inside RANS (SAS) zone at $X^* = 0.6$ (just after LES zone).

Figure 14. Backward facing step RANS (RSM). Viscosity ratio on isosurfaces of q-criterion ($\leq 2000$).

Figure 15. Backward facing step RANS (SAS). Viscosity ratio on isosurfaces of q-criterion ($\leq 2000$).