INTRODUCTION

Applied large eddy simulation

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Large eddy simulation (LES) is now seen more and more as a viable alternative to current industrial practice, usually based on problem-specific Reynolds-averaged Navier–Stokes (RANS) methods. Access to detailed flow physics is attractive to industry, especially in an environment in which computer modelling is bound to play an ever increasing role. However, the improvement in accuracy and flow detail has substantial cost. This has so far prevented wider industrial use of LES. The purpose of the applied LES discussion meeting was to address questions regarding what is achievable and what is not, given the current technology and knowledge, for an industrial practitioner who is interested in using LES. The use of LES was explored in an application-centred context between diverse fields. The general flow-governing equation form was explored along with various LES models. The errors occurring in LES were analysed. Also, the hybridization of RANS and LES was considered. The importance of modelling relative to boundary conditions, problem definition and other more mundane aspects were examined. It was to an extent concluded that for LES to make most rapid industrial impact, pragmatic hybrid use of LES, implicit LES and RANS elements will probably be needed. Added to this further, highly industrial sector model parametrizations will be required with clear thought on the key target design parameter(s). The combination of good numerical modelling expertise, a sound understanding of turbulence, along with artistry, pragmatism and the use of recent developments in computer science should dramatically add impetus to the industrial uptake of LES. In the light of the numerous technical challenges that remain it appears that for some time to come LES will have echoes of the high levels of technical knowledge required for safe use of RANS but with much greater fidelity.

Keywords: large eddy simulation; boundary conditions; initial conditions; best practice; hybrid RANS–LES

1. Introduction

Industrial flows are physically complex, highly unsteady, and have large Reynolds number. This means a substantial scale separation between the large, energy containing, structures and the small, dissipative, scales. Until

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recently, the only tenable approach to industrial practice was based on the Reynolds-averaged Navier–Stokes (RANS) models, for which only averaged information can be obtained. While (unsteady) RANS methods will still be widely used in industry for many years to come, large eddy simulation (LES) is now mature enough to be used for the analysis of specific problems; particularly aspects of external aerodynamics of trains and cars (Krajnović 2009), in turbomachines (Eastwood et al. 2009; Menzies 2009), for weather forecasting (Cullen & Brown 2009) and characterizing flow mixing processes (Youngs 2009).

These problems are very different from one to another, hence requiring different, ad hoc, RANS models. On the other hand, they present significant similarities which make them suitable for LES modelling. For example, these flows are primarily driven by large-scale structures, which are affected by unsteady heat transfer and complex geometries, and those characteristics can be more easily modelled using a time-filtered approach rather than the RANS time-averaged approach.

However, the range of scales to be modelled in an atmospheric boundary layer is orders of magnitude higher than that in a turbomachine. In the first case (weather forecasting), the flow is strongly dependent on initial local flow conditions gained through observation and LES is used as a predictive tool in an extrapolative sense. In the second case (turbomachine), there is minimal information about the flow itself, and LES is sought to replace experiments in understanding the flow physics, and will ultimately be used to help improve component design. Compared to RANS, the advantages of LES are important. RANS methods have a well-known limited range of applicability, and their performance needs to be thoroughly assessed by comparison to measurements. Even then, the uncertainty associated with RANS methods is high, whatever the method is. Moreover, for many unsteady flows, the assumption behind the calibrations of most RANS equations (e.g. time averaging versus ensemble averaging) becomes questionable. LES does not have these issues: all scales (down to the cut-off wavelength) are fully resolved, and the smallest ones are expected to have only a weak relationship with the big, energy-containing scales (and their effects can be ‘averaged’).

Nevertheless, generalization of LES methods to industry, where geometries are complex and Reynolds numbers generally high, is still problematic, for example needing greater elements of approximate modelling. First, as with RANS, the performance will depend albeit in a diluted sense on the choice of model. At very high Reynolds number, with the presence of walls, hybrid methods, bringing in a near-wall RANS element, such as DES (Strelets 2001) or seamless models (§2), seem to be the most promising (in terms of cost versus accuracy; Leschziner 2009). Further from the wall, and using appropriate numerical schemes, implicit LES (ILES) is an attractive alternative (Margolin 2009). With this, no explicit (LES) model is used but the inherent numerical scheme traits/errors are used to implicitly replace the LES model.

A challenge in running a good simulation (even RANS simulations) is to prescribe the ‘right conditions’ (e.g. similar boundary and initial to that of the experiment). There are already a large number of publications addressing the issues associated with LES modelling (e.g. Pope 2004). Here, we will try to address those most relevant to industry, for which maximum efficiency is more
often sought than maximum accuracy (i.e. obtaining the right balance between numerical accuracy and cost). More specifically, there are three important questions that need to be answered.

— What must be done at the subgrid scale (SGS) level?
— What must be done close to a wall?
— What must be done at the boundaries (other than walls)?

These are indicated in figure 1 and each of them will be addressed in the following sections. The answers to the questions are far from trivial, and have been the main topic of most of the papers presented at the Royal Society discussion meeting on LES. Beside these three questions, there are also other practical issues that need to be addressed, to obtain a credible degree of confidence from LES results.

— What level of detail do I need from my simulations?
— How should they be validated?

The last question, especially, is crucial as it also implies improvement of experimental techniques and this will be dealt with in §6.

It also reflects that bringing LES to fruition needs input from multiple communities.

### 2. Subgrid-scale modelling

The number of LES models has increased almost exponentially in recent years. A non-exhaustive list of models and their variants can be found in Sagaut (2006). Interestingly, and very much like in the RANS community, in which the original $k-\varepsilon$ and the more recent $k-\omega$ models are the most widely used, only a handful of SGS models are being used in practice: the original Smagorinsky model (analogous to the simplest RANS mixing length model, the modelled length scale based on cell size rather than wall proximity) being favoured in a large
majority of cases. Hence, the question arises about the effort expended to develop new SGS models, and if this effort would not be better used in other areas (Hutton 2009). Indeed, recent work (Grinstein et al. 2007) has shown that ILES (no model) is adequate or even sometimes preferable.

Also, since for LES, the SGS model should only account for a small percentage of the turbulence energy, there is the question of priorities, especially for industrial practice. For example, in focusing too heavily on the SGS model, do we miss aspects of more substantial impact, such as problem definition? Hence, the ingredients that have the greatest solution impact need to be prioritized. This aspect was partly considered by Eastwood et al. (2009).

Indeed, an important problem in turbulent flow simulations is that, counter-intuitively, not all flows are turbulent all the time. The flow can relaminarize when subjected to favourable pressure gradient or it can have a significant portion of the flow laminar before transitioning to turbulence (e.g. bypass transition—see §5). In non-turbulent regions, the SGS model should be deactivated, or should ‘react’ in the right way. So far, this problem has attracted very little attention, and some works are only trying to address the problem using conventional approaches: the Lagrangian dynamic model (Meneveau et al. 1996) for instance is suited for this purpose, but remains computationally expensive. For other methods, such as RANS hybridizations (§4), dealing with laminar flow zones is especially unclear (Eastwood et al. 2009).

In many industrial applications the turbulence may be the primary driver, but other important SGS phenomena must be correctly resolved or even modelled. Aeroacoustic (Sagaut & Deck 2009), mixing (Youngs 2009), chemical reaction (Fureby 2009) are of primary interest in many industrial applications, and are dependent both on the right description of the large scales, and also on the small-scale behaviour (e.g. mixing).

These additional SGS explicit issues do not preclude the use of ILES. For example, in the work of Fureby (2009), SGS parametrization of combustion is hybridized with ILES. Indeed, as pointed out by Geurts (2009) numerical influences/errors are extremely hard to eradicate (theoretically impossible with a second-order scheme and standard LES filter) but can assist in gaining more accurate solutions. Hence, for industrial LES it would not seem unreasonable to turn this negative discretization error aspect to advantage. This could be done through use of code-customized LES models where, if possible, classical LES model terms are judiciously selected to enhance SGS analogous terms already mimicked by the discretization, i.e. hybrid LES–ILES. The work of Fureby (2009) carries the concept of hybridization further by including a third ingredient—the log-law wall-function used for RANS modelling. Hence, these simulations could be viewed as having faint echoes of hybrid ILES–LES–RANS modelling. The hybridization of RANS with (I)LES will be discussed later.

3. Numerical discretization

Another aspect, linked to the above and very important for industrial practice, is related to discretization. Indeed, from a practical perspective, this can define the appropriate SGS model and whether it is implicit or explicit. For a neutrally dissipative solver an implicit SGS model is mandatory. However, as
demonstrated by Ghosal (2002) and Chow & Moin (2003), for a second-order scheme and standard filter the numerical influence will dominate the SGS making it hard to conceive how, if there was the perfect SGS model, it could be correctly used. With increasing dissipation (this can arise in the solution from multiple sources) the appropriate SGS modelling strategy becomes even less clear partly prompting the frequent LES versus ILES debate. For very complex engineering problems, complex grids are required, and the easier option is to use unstructured meshes that preclude the use of higher order upwinding. Most recent commercial packages (FLUENT or STARCCM) also use polyhedral meshes. This has to be related to the SGS model in some way, and this also requires specific attention from practitioners. As shown by Tucker (2008), cell topology can have a dramatic numerical influence in the context of resolving turbulent flow features. Indeed, cell topology introduces additional terms that become apparent through use of modified equation analysis. These terms will make SGS level contributions. Hence, numerical discretization is a problematic area for both the ILES and LES communities and, as ever, the temporal discretization should not be neglected and its influence again explored through modified equation analysis. Typically, classical ILES uses high-order upwind schemes for compressible flow on structured grids. However, the stencil flipping for such schemes around flow symmetries can introduce artificial flow instability. Also, we note here that the numerical discretization and grid are closely coupled and it is necessary to know how a particular grid will react with a particular solver. The numerous discretization issues did not feature as prominently at the meeting as they might have done. This perhaps partly reflects the relatively benign geometries considered and hence the status of applied LES. However, as pointed out by Krajnović (2009), geometric complexity can frequently also alleviate modelling challenges—the features removing the expensive-to-compute classical boundary-layer content.

4. Near-wall modelling

There is another important modelling aspect which needs careful attention. The treatment of near-wall behaviour is crucial in many configurations (that is where, most often, the turbulence is produced) and requires specific modelling. Indeed, a whole class of models have been developed to address this particular problem. The main issue is that, as the distance from the wall reduces, so does the integral scale, hence requiring a resolution increase. The resolution increases linearly with the Reynolds number and the problem becomes far too expensive (e.g. Piomelli & Balaras 2002). Specific models have been developed to maintain a relatively low-cost simulation while allowing high Reynolds numbers to be reached. The most classical approach is to use a wall-model (e.g. a popular wall-model, available in many commercial packages, was proposed by Werner & Wengle (1991)).

Alternative more RANS centred methods have been introduced: DES (cf. review from Strelets (2001) and Spalart (2009)), hybrid RANS–LES (Piomelli & Balaras 2002) and zonal RANS–LES (Tessicini et al. 2007), each of them introducing a bridge between a near-wall RANS-like approach and a LES-like behaviour further from the wall. For the first method (DES), the
bridging is continuous (seamless method), but the unsteady part of the solution is dependent on the grid size (Spalart et al. 2006). For other (discrete) blending methods, the interface between a near-wall RANS layer and the LES region, away from the wall, is usually fixed, ideally requiring a correct prescription of the fluctuations from the RANS to the LES part (generation of synthetic turbulence) and a filtering of the information coming from the LES part to the RANS wall-layer. Possible treatment of that interface is the focus of papers from Davidson (2009) and Leschziner (2009).

A key aspect of the discussion meeting was that although ILES had clearly become accepted by many participants, feelings became more raw in relation to ILES use near walls. Solid connections can be drawn between classical LES modelling and the numerical discretization terms used by ILES. This is an argument used to justify ILES. However, this being the case ILES should, as LES, become problematic near walls where at high Reynolds number grid resolution demands are severe. Hence it seems unclear why the LES community has invested substantial research effort into hybridization with near-wall RANS modelling and the ILES community has not considered this technique. There seems three possible reasons for the success of pure ILES for wall bounded flows:

— some ILES are akin to wall resolved LES, i.e. they are quasi-direct numerical simulation (DNS) near walls (Drikakis et al. 2009);
— some form of wall modelling is used, such as log-wall functions, but the use and justification of the actual ILES approach detracts attention from the fact that there is wall treatment (Fureby 2009); and
— some flows considered are more ‘top-down’ than ‘bottom-up’.

By the former, it is meant that turbulent structures external to the wall region are strongly convected into the boundary layer. The structures overwhelm the classical boundary-layer physics. Under these circumstances the importance of the wall modelling is diluted. Examples of this would be the combustion modelling work of Fureby (2009) and perhaps turbomachinery flows with multiple stages. Then the wakes from upstream blade rows will impact on the boundary layers of downstream blade rows (where such zones can be defined—in many complex flows the near-wall flow physics being quite unlike that of a classical boundary layer).

5. Boundary and initial conditions

In LES, canonical spatially evolving flows are sometimes temporally evolved. This avoids the need for complex time evolving boundary condition specifications. Hence, initial and boundary conditions can be inter-related and this connection came across at the meeting. The explosive (Youngs 2009) and meteorological flows (Cullen & Brown 2009) are highly dependent on initial conditions and the turbomachinery (Eastwood et al. 2009) potentially dependent on upstream boundary conditions.

The meeting identified that frequently the most important aspect of unsteady simulations, should it be DNS, LES or hybrid RANS–LES, is the need for accurate unsteady boundary conditions, both at the inlet and at the RANS–LES interface. The issues associated with interface conditions between a RANS and an LES
region have already been mentioned in §4. Inflow condition (and associated with it are the initial conditions) is crucial to get the right flow field for many practical flows. It has been shown that the whole flow behaviour can be sensitive to the inflow, and that the memory effect can be important (Grinstein 2009), even at high Reynolds number.

There are several aspects that need to be considered when generating inflow conditions. First, the spectral content (down to the cut-off wavenumber) must be prescribed in instantaneous ways. Several methods have been developed, the most common one, used in boundary layer flows, is the recycling method (Lund et al. 1998). For other cases, one can reconstruct the flow field based on measurements (or from other simulations) using a combination of linear stochastic estimation and principal component analysis (Druault et al. 2004). This technique can be applied for instance for weather forecasting, for which data are available at a given discrete number of locations in space. Second, the dependence on initial conditions should be assessed. If the flow displays a bi-stable mode for instance (e.g. pair of cylinders in flapping regime; Kim & Durbin 1988), one might get only one of two possible solutions during the simulated period, advocating for a return to the ensemble average rather than rely only on time-averaging. Finally, the flow-behaviour dependence for slight changes in mean and spectral flow content should be studied, for validation with experiments. However, such studies are expensive: because the flow adapts only slowly to the condition, a significant portion of the domain is dedicated to physically unrealistic behaviour, hence increasing the cost of the computation.

Note that grid, SGS model and numerics are all closely coupled to the inflow boundary condition. If these elements will not accurately support the imposed inflow turbulence, accurate inflow specification is futile. Indeed the subject of inflow alone would make a valuable theme for a scientific meeting.

6. Validation and measurements

An important asset of LES for industrial applications is to generate more spatial, temporal and structural detail than RANS allows. However, the question for industry is to know what data are relevant to them. In some cases, if only integral quantities (e.g. lift, drag) are needed, a switch to LES may be undesirable, given the cost increase. Some RANS models, used wisely, are more likely to give a useful answer quickly. This can also be related to another problem: how do we validate LES (beyond classical integral parameters)? Sagaut & Deck (2009) proposed six levels of validation, and out of them three are specific to LES (and DNS) methods. Assessing the degree of confidence of the quantities considered is vital to avoid misinterpretations.

Primarily through George & Tutkun (2009) the need emerged for canonical flow datasets at sufficiently high Reynolds number where, for example, boundary layers are truly turbulent. Related to this is the danger of placing too much emphasis on the use of relatively low Reynolds number DNS data for validation and model development purposes. Also, as ever, there is the pressing need for high quality data for realistic industrial geometries with well defined boundary conditions having representative auxiliary flow physics (e.g. combustion influences). Also, measurements should be put to greater specific use in

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informing modelling practice and numerical model refinement. For example, measurements could be used to help classify top-down, bottom-up and mixed regime flows and hence the development of hybrid LES–RANS methods.

Experimentalists are beginning to grapple with repeatability. By this it is meant that the flow can vary from one experimental run to another. For example, shock location can vary by approximately 20 per cent of chord between experiments. This presents difficult issues for both the measurement and LES communities in dealing with such uncertainties. This is especially the case for LES users where run times are (compared to measurements) vast. We note here that boundary conditions are not just the bane of LES modellers. With experiments, although precise measurements are made, the true nature of the system being studied is seldom clear.

7. Conclusion

LES in the near future will be a real alternative to RANS. There is little doubt about this, and a lot of effort has been expended making LES, DES and other hybrid methods more robust for industrial use. Indeed, most CFD packages (FLUENT, StarCCM, etc.) now include by default LES options (even sometimes DNS). However, careful attention needs to be paid to knowledge transfer, and we should learn from some of the mistakes encountered when RANS was introduced into industry, and an awareness of the limitations of LES is needed. For this purpose Hutton (2009) rightly advocates the development of best practices guidelines. However, these should not detract from the fact that the safe use of LES needs a level of fundamental understanding.

Again, LES should be seen as a complementary tool to experiments, and will not, in the foreseeable future, replace testing, and industrial practitioners should be aware of those limits. Indeed, a closer collaboration between experimentalists and numericists is required both for developing accurate tools and for using them to their full potential.

The need for more careful characterization of experimental/numerical boundary and initial conditions was illustrated in many of the meeting papers.

There was the feeling that for LES to make most speedy industrial impact, pragmatic hybrid use of LES, ILES and RANS elements will probably be needed. Added to this further, highly industrial sector SGS model parametrizations will be required with clear thought on the key target design parameter(s). The meteorological office work of Cullen & Brown (2009) contained echoes of this philosophy, their work being driven by the pressing need for reliable forecasts in acceptable time frames. The combination of good numerical modelling expertise, a sound understanding of turbulence, along with artistry, pragmatism and the use of recent developments in computer science (allowing parallel pre- and post-processing along with harnessing, for example, more exotic processor architectures such as GPUs) should dramatically add impetus to the industrial uptake of LES. Grid generation is as ever a CFD bottleneck (in terms of an engineer’s time) and LES places special demands on grid generation. This seems an area where initial best practice guidance would be especially welcome, the grid defining very much both the explicit LES modelling requirements and also many implicit modelling elements.
In the light of the numerous technical challenges that remain in terms of boundary conditions, grid generation, numerical schemes, SGS modelling, problem and filter definition and the complex interaction between these elements it appears that for some time to come LES will have echoes of the high levels of technical knowledge required for safe use of RANS.

References


