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REVIEW ARTICLE

Large-eddy simulation: Past, present and the future (crossMark



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Abstract Large-eddy simulation (LES) was originally proposed for simulating atmospheric flows in the 1960s and has become one of the most promising and successful methodology for simulating turbulent flows with the improvement of computing power. It is now feasible to simulate complex engineering flows using LES. However, apart from the computing power, significant challenges still remain for LES to reach a level of maturity that brings this approach to the mainstream of engineering and industrial computations. This paper will describe briefly LES formalism first, present a quick glance at its history, review its current state focusing mainly on its applications in transitional flows and gas turbine combustor flows, discuss some major modelling and numerical challenges/issues that we are facing now and in the near future, and finish with the concluding remarks. © 2015 Production and hosting by Elsevier Ltd. on behalf of CSAA & BUAA.

1. Introduction

Almost all practical engineering and the vast majority of naturally occurring flows are turbulent and hence the focus of research in computational fluid dynamics (CFD) is devoted to flows in which turbulence plays a dominant role. Although the exact physical nature of turbulence has not been fully understood, it can be modelled to a sufficient degree of accuracy in numerical simulations.

Turbulence is always three-dimensional (3D) and unsteady with a large range of scale motions. As a result of this the primary problem with numerically computing (as well as measuring) turbulence is the enormous range of scales that must be

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resolved. The size of the computational domain must typically be at least an order of magnitude larger than the scales characterising the turbulence energy while the computational mesh must be fine enough to resolve the smallest dynamically significant length-scale (the Kolmogorov micro-scale) for accurate simulation. The most accurate approach for simulating turbulent flows is called the direct numerical simulation (DNS) in which the full Navier-Stokes equations are numerically solved directly using very fine mesh to capture all the scales that are present in a given flow, from the smallest to the largest eddies. Therefore computationally DNS is very expensive and at present it can be applied only to low Reynolds number flows over simple geometry.

In some cases, one is mainly interested in the steady-state fluid flow and hence it is not necessary to simulate the detailed instantaneous flow, leading to a great reduction of computational time. This is the basis for the Reynolds-averaged Navier-Stokes (RANS) approach in which one solves only for the averaged quantities while the effect of all the scales of instantaneous turbulent motion is modelled by a turbulence model. This approach has been the backbone in the industrial

CFD applications for the last few decades due to its modest computing requirement. Nevertheless knowledge of the transient behaviour of the flow is necessary and the RANS approach is therefore not sufficient and in many cases it fails to predict the flow behaviour such as transition.

An alternative approach is called large-eddy simulation (LES) which was proposed in as early as 1963 by Smagorinsky. LES does not adopt the conventional time- or ensemble-averaging RANS approach with additional modelled transport equations being solved to obtain the so-called Reynolds stresses resulting from the averaging process. In LES the large scale motions (large eddies) of turbulent flow are computed directly and only small scale (sub-grid scale (SGS)) motions are modelled, resulting in a significant reduction in computational cost compared to DNS. LES is more accurate than the RANS approach since the large eddies contain most of the turbulent energy and are responsible for most of the momentum transfer and turbulent mixing, and LES captures these eddies in full detail directly whereas they are modelled in the RANS approach. Furthermore the small scales tend to be more isotropic and homogeneous than the large ones, and thus modelling the SGS motions should be easier than modelling all scales within a single model as in the RANS approach. Therefore, currently LES is the most viable/promising numerical tool for simulating realistic turbulent/transitional flows.

This paper presents briefly LES formalism first followed by the following sections: a short introduction to the history of LES and its development, a brief review of the present position of LES focusing mainly on its applications in aeroengine related flows, the major challenges/issues of LES and concluding remarks.

The review in this paper is mainly limited to the traditional LES and will not review other approaches under the LES umbrella such as ILES (Implicit LES) or called MILES (Monotone Integrated LES), VLES (Very LES) and the hybrid LES/RANS approach. The author would like to declare that this review is by no means inclusive as it is impossible to include every piece of work published in this area and many points presented in this paper only reflect the author's personal opinion.

2. Mathematical formulation

2.1. LES governing equation

The governing equations, called the Navier–Stokes equations, are derived from the fundamental conservation laws for mass, momentum and energy. In LES only large eddies (large scale motions) are computed directly and hence a low-pass spatial filter is applied to the instantaneous conservation equations to formulate the 3D unsteady governing equations for large scale motions. This is called explicit filtering and Fig. 1 illustrates the difference between the filtered velocity \bar{u}_i and the instantaneous velocity u_x .

When the finite volume method is employed to solve the instantaneous governing equations numerically the equations are integrated over control volumes, equivalent to convolution with a top-hat filter, therefore there is no need to apply a filter to the instantaneous equation explicitly and this is called implicit filtering. However, it is worth pointing out that there

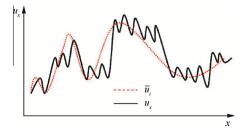


Fig. 1 Difference between the filtered velocity and the instantaneous velocity.

is potentially a big shortcoming or pitfall in implicit filtering, i.e., a truly mesh independent results can never be achieved as with the refinement of mesh, smaller scale motions are resolved and if one keeps on refining the mesh then eventually a DNS is performed, not an LES. In other words, when implicit filtering is employed it is almost impossible to distinct between numerical and modelling errors and hence prohibits useful analysis of numerical schemes.

The filtered equations expressing conservation of mass and momentum in a Newtonian incompressible flow can be written in conservative form as

$$\partial_i \bar{u}_i = 0 \tag{1}$$

$$\partial_t(\rho \bar{u}_i) + \partial_i(\rho \bar{u}_i \bar{u}_i) = -\partial_i \bar{p} + 2\partial_i(\mu \bar{S}_{ij}) - \partial_i(\tau_{ij})$$
 (2)

$$\overline{S_{ij}} = \frac{1}{2} (\partial_i \overline{u_j} + \partial_j \overline{u_i}) \tag{3}$$

$$\tau_{ii} = \rho(\overline{u_i u_i} - \overline{u_i} \overline{u_i}) \tag{4}$$

where ρ is density; \bar{u}_i is filtered velocity; \bar{p} is filtered pressure; μ is molecular viscosity; \bar{S}_{ij} is the filtered, or resolved scale strain rate tensor and τ_{ij} is the unknown SGS stress tensor, representing the effects of the SGS motions on the resolved fields of the LES, which needs to be modelled using a so-called SGS model so that the above governing equations can be solved.

2.2. SGS modelling

Many different kinds of SGS models have been developed^{2–5} and most of them make an eddy-viscosity assumption (Boussinesq's hypothesis) to model the SGS stress tensor as follows:

$$\tau_{ij} = 2\mu_t \overline{S_{ij}} + \frac{1}{3} \delta_{ij} \tau_{ll} \tag{5}$$

where μ_t is called SGS eddy viscosity and substitute this into Eq. (2) which then becomes

$$\partial_t(\rho \bar{u}_i) + \partial_i(\rho \bar{u}_i \bar{u}_j) = -\partial_i \bar{p} + 2\partial_i [(\mu + \mu_t) \bar{S}_{ij}] \tag{6}$$

Note that a modified pressure $\overline{P} = \overline{p} + \frac{1}{3}\tau_{ll}$, has been introduced and as a result of this when the above equation is solved the pressure obtained is not just the static pressure only. The remaining problem now is how to determine the SGS eddy viscosity and the most basic model is the one originally proposed by Smagorinsky:¹

$$\begin{cases} \mu_{t} = \rho \left(C_{S} \overline{\Delta} \right)^{2} S \\ S = \left(2 \overline{S}_{ij} \overline{S}_{ij} \right)^{\frac{1}{2}} \\ \Delta = \left(\Delta x \Delta y \Delta z \right)^{\frac{1}{3}} \end{cases}$$

$$(7)$$

where $C_{\rm S}$ is the so-called Smagorinsky constant which depends on the type of the flow, e.g., the value of 0.18 gives reasonable results for isotropic turbulence whereas for flows near a solid wall it should be reduced to 0.1.

Although much efforts have been made in developing more advanced SGS models and there are many SGS models available, this very simple model is still used and proved surprisingly successful. Nevertheless it is well-known that this model has clear shortcomings such as too dissipative (not good for transition simulation) and the Smagorinsky constant needs to be adjusted for different flows. One way to avoid adjusting the constant artificially and hence to improve this simple SGS model was suggested by Germano et al. 6 – a dynamic SGS model, allowing the model constants $C_{\rm S}$ to be computed locally in space and in time during the simulation. More discussion and review of SGS models can be found elsewhere. $^{7-16}$

2.3. Numerical methods

The finite volume method has become the most popular numerical method for LES and when this numerical method is employed it is not necessary to apply a filter to the instantaneous equation explicitly, hence called implicit filtering as discussed in Section 2.1 so that filtering will not be discussed anymore in this section. There are still many other numerical issues in LES but in this section only a very brief discussion on spatial and temporal discretization will be presented and more discussion will be focused on the generation methods for the inflow boundary conditions.

2.3.1. Spatial and temporal discretization

One of the most popular spatial discretization scheme used in LES is the second-order central difference because it is non-dissipative and conservative (not only mass and momentum but also kinetic energy conserving), which are essential for LES. Usually, first- and second-order upwind schemes or any upwind-biassed schemes are not used in LES since they produce too much numerical dissipation. While higher-order numerical schemes, generally speaking, are desirable and can be applied fairly easily in simple geometries, their use in complex configurations is rather difficult. Hence it is likely that with increasing applications of LES to flows of engineering interest in complex geometries the second-order central difference scheme is still going to be wisely used.

As for the temporal discretization (time advancement), implicit schemes have the advantage of using larger time steps. Nevertheless, they are more expensive computationally to solve the governing equations at each time step compared against explicit schemes. Furthermore, large time steps are unlikely to be used in LES in order to resolve important time scales of turbulence. Therefore, explicit schemes seem to be more suitable for LES than implicit schemes and most researchers in LES use explicit schemes such as the second-order Adams–Bashforth scheme. Since the time steps are usually small in LES, it is not essential to use higher-order temporal schemes either.

2.3.2. Inflow boundary conditions

Boundary conditions are very important in any numerical simulations and this is particularly true for LES. Among all the boundary conditions the most important one is how to specify inlet boundary conditions accurately because the downstream flow development within the domain is largely determined by the inlet behaviour in many cases. Nevertheless, it is an extremely difficult task to generate inlet boundary conditions accurately in LES because, unlike the RANS computations where only time-averaged information is required, in LES three components of instantaneous velocity need to be specified at each time step, which should possess characteristics such as stochastically varying, with scales down to the filter scale (spatially and temporally), compatible with the Navier-Stokes equations, turbulent structures (turbulence intensities, length scales, spectrum etc.). Therefore it is extremely hard, if not impossible, to generate inlet boundary conditions in LES which have all the listed characteristics above. In particular it is possible to generate a wide range of flow fluctuations around the mean which may have specified spectral properties such as intensity and length scales, and even compatible with the Navier-Stokes equations. However those generated flow fluctuations may not have the structure of turbulence, i.e., coherent eddies across a range of spatial scales down to the Kolmogorov scale which interact with each other. In addition it is also worth pointing out that turbulent structures are different between free-stream turbulence and wall-bounded turbulence and so on.

Generally speaking, current inflow boundary condition generation methods in LES can be classified into two basic categories: the so-called "precursor methods" in which an addition simulation (precursor simulation) is performed and the required data are stored as the input for the required simulation, and "synthesis methods" in which some form of random fluctuation is generated/manipulated and combined with the given mean flow at the inlet. Precursor methods can generate the most realistic turbulence information at inflow boundary but the disadvantage is the necessity to set up and run a separate calculation, leading to usually very high computational cost. One way to save the computational cost is to integrate the precursor calculation into the main domain, with data downstream of the inlet being mapped back into the inlet. It is of course necessary to provide some mechanism for driving the flow towards a pre-specified target such as mean velocity profiles and turbulent stresses etc. by recycling and rescaling. This method, which was first developed for flat-plate boundary layers, consists of taking a plane of data from a location downstream and rescaling the inner and outer layers of velocity profiles separately, to account for the different similarity laws that are observed in these two regions. The rescaled velocity profiles are then reintroduced at the inlet. The main shortcoming is that the inlet must be placed in a region in which the flow is in an equilibrium or very slowly developing, well-known condition (mean velocity and turbulent quantities) and a fairly long domain must be used for the region of interest for the recycling.

Many synthesis generation methods have been developed and the simplest way is to specify the mean flow velocity profile plus some kind of random perturbations, e.g., adding a white-noise random component to the mean velocity at inlet, with an amplitude determined by the turbulent intensity level. This method is very easy to implement but not a good one at all since the white noise component has hardly any of the required characteristics of turbulent flow – in particular it possesses no spatial or temporal correlations at all. Therefore, they decay

rapidly and it takes usually a long distance downstream from the inflow boundary for a desired realistic turbulence to develop, and in some cases the use of random noise at the inlet does not develop turbulence downstream at all. Over the past decades significant efforts have been made to develop advanced synthesis techniques generating fluctuations which are more realistic with required spatial and/or temporal correlation. Available advanced synthesis generation methods can be broadly classified into four categories: Fourier techniques¹⁷ and related approaches, proper orthogonal decomposition (POD) methods, 18 digital filter generation methods 19 and finally vortex method²⁰ or synthetic eddy method (SEM). Details on inlet boundary condition generation methods can be found in a review article.²¹ Nevertheless, all those advanced synthesis methods mentioned above can only generate inflow turbulence with certain properties and no methods available yet to generate inflow turbulence with all the desired characteristics such as turbulence intensity, shear stresses, length scales, power spectrum and proper turbulent structures as mentioned previously.

3. A very brief history of LES and its development

LES was first proposed in 1963 by Smagorinsky¹ for atmospheric flow prediction and the early applications were also in this area.²²⁻²⁴ LES was first applied to engineering related flow by Deardoff in 1970²⁵ and by Schumann in 1975.²⁶ The initial development of LES from the 1960s to about middle of the 1980s was slow and the applications were mainly simple, building-block flows: homogeneous turbulence, mixing layers, plane channel flows and so on. However, with the increase of computing power a very rapid development and sharp increase in applications of LES started from about middle of the 1980s, especially after the 1990s with significant growth of LES community and a wide range of applications of LES shifting from simple flows to complex flows including multi-phase flow, heat transfer, combustion, aeroacoustics etc. Apart from the increase in computing power one major factor behind such rapid development and wide range of applications of LES is because it has become clear that RANS methods inherently cannot handle certain classes of complex turbulent flow problems.

The development and growing interest towards LES is clearly indicated by several distinct factors. Firstly, the number of articles published annually in international journals. Secondly, in parallel to this tremendous increase in journal publications, a noticeable increase in the number of contributed talks in international conferences. Thirdly, a very significant increase of LES research groups/people across the world. Fourthly LES becomes available in most commercial CFD software. Finally, many monographs dealing specifically with LES have been published.^{3,27–37}

4. Current state of LES

As mentioned in the above section, during the early period of LES applications it was used successfully to investigate the details of flow problems having relatively simple geometry and at low Reynolds numbers such as homogeneous turbulence, mixing layers, plane channel flows. Although use of LES in such an academic or fundamental setting continues

today mainly for model validation and fundamental understanding of flow physics etc. emphasis has shifted to more complex configurations having flow characteristics where the RANS approach has failed. In particular, after several decade's development in LES and the availability of massively parallel computers and affordable workstation clusters have stimulated industry interest in applying LES to complex engineering flows. Nevertheless LES has not replaced the RANS approach and will not replace it for the near future to become the main computational analysis tool for practical engineering problems due to two main reasons: firstly, even with the current computing power it is still far too expensive computationally to perform LES on a routine basis for practical engineering flow problems; secondly, LES has not reached such a level of maturity that users without significant experience and knowledge can obtain results with the level of solution fidelity that can be expected. For the foreseeable future LES will not become a design tool that can be employed by persons without extensive years of experience on LES techniques.

In this section a brief review of LES applications in transitional flows and gas turbine combustor flows will be given to illustrate the current state of LES rather than a precise summary of the current capabilities of LES, which is extremely hard, if not impossible.

4.1. LES of transitional flows

Earlier numerical simulations were mainly focused on understanding transition mechanisms of flows with simple geometry and there were much fewer LES studies of transitional flows compared with DNS studies (especially for natural transition where it is essential to capture the instabilities involved) because of concerns about the penalties arising from low resolution and SGS modelling such as the Smagorinsky model which is too dissipative for natural transition simulation. However, Ducros et al.³⁸ demonstrated that with a proper SGS model LES could be used to simulate natural transition successfully and the SGS model used in their study is called the filtered-structure-function (FSF) model. Details of a natural transition process was also captured correctly in an LES by Huai et al.³⁹ using a localised dynamic SGS model. Recently Sayadi and Moin⁴⁰ carried out a detailed study to assess the performance of several SGS models in predicting natural transition.

Bypass transition appears to be different since the transition is early and short so that the detailed computation of the form of the instabilities is not crucial as shown for the first time by Yang et al.41-43 using a modified Smagorinsky SGS model to allow for the very low Reynolds number of the flow. The effects of a high free-stream turbulent field on a spatially evolving boundary layer was investigated using LES with a dynamic mixed SGS model and bypass transition was observed giving rise to mechanisms of turbulent energy production.⁴⁴ LES of bypass transition along a flat plate was carried out using an SGS model constructed based on variational multiscale concepts⁴⁵ and the results agreed well with the DNS data. LES of bypass transition for different sets of free-stream turbulence conditions with a localised Lagrangian-averaged dynamic SGS model was performed by Lardeau et al. 46 to address mainly the evolution of the budgets, with particular

attention focusing on shear production relative to pressure–velocity interaction performed.

LES has also been successfully applied to investigating transitional separated flows^{47–57} and is still applied currently to this kind of fundamental research such as separated boundary layer transition under elevated free-stream turbulence level by Langari and Yang.⁵⁸ Fig. 2 shows the computational domain and mesh used in Langari and Yang's study.⁵⁸ Using

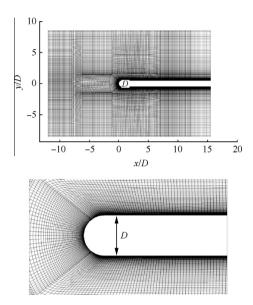


Fig. 2 Computational domain and mesh. 58

the multi-block functionality, the domain is divided into 14 blocks with a grid resolution of $(n_x, n_y, n_z) = (310, 140, 64)$ for the outer region and a refined C-grid (420, 60, 64) around the plate covering the close wall region and the free shear layer region of the separation bubble, a total of 4.39 million mesh points. Figs. 3 and 4 present the comparison between the predicted mean streamwise velocity U and RMS (Root Mean Square) of streamwise velocity fluctuation u' normalised by the inlet velocity U_0 of fluctuations with the experimental data (where l is the mean separation bubble length). As can be seen from both figures that an excellent agreement has been obtained between the predicted mean profiles and the experimental data at all locations. The predicted RMS of streamwise velocity fluctuations compare very well with the experimental data in terms of both peak values and their locations.

Fig. 5 shows the flow structures under very low free-stream turbulence and elevated free-stream turbulence level of 5.6%. For the very low free-stream turbulence case the spanwise oriented quasi-2D Kelvin–Helmholtz (KH) rolls are clearly visible at the early stage of the bubble and then become distorted/deformed due to 3D motion setting in as a result of a possible secondary instability. However, for the elevated free-stream turbulence case those spanwise oriented quasi-2D KH rolls are not visible and spanwise irregularity appears at the early stage of the bubble in the separated shear layer leading to the formation 3D hairpin like structures, bypassing the stage where the quasi-2D KH rolls exist, leading to a much earlier breakdown to turbulence, similar to the "bypass transition" process in attached boundary layers where TS instability stage is bypassed.

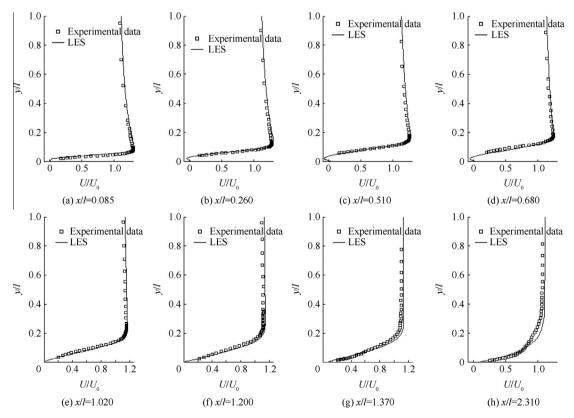


Fig. 3 Comparison of predicted mean streamwise velocity at different streamwise stations with experimental data. 58

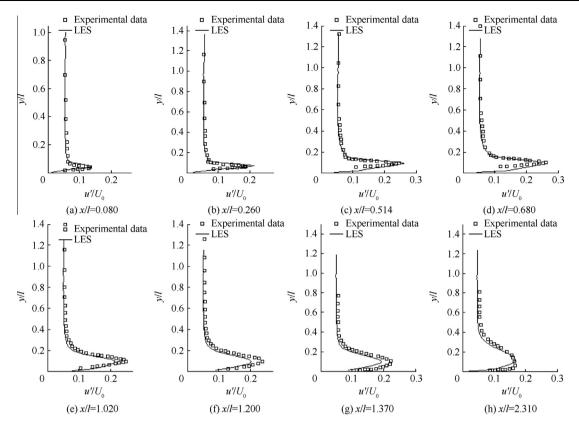


Fig. 4 Comparison of predicted RMS of streamwise velocity fluctuation at different streamwise stations with experimental data.⁵⁸

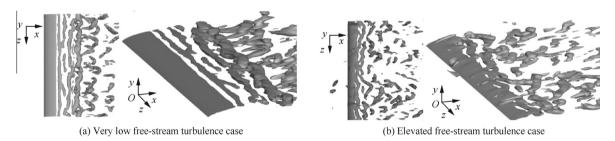


Fig. 5 Top and perspective views of the Q-criterion iso-surfaces showing flow structures⁵⁸.

It is much hard to simulate transition in realistic engineering flow cases as apart from the geometrical complex the flow is also very complex with many factors influencing the transition process: pressure gradients, Reynolds number, curvature, level and scale of turbulence, roughness, unstationarity etc. Nevertheless applications of LES to study transition in realistic engineering flow cases have started appear such as transitional flows over turbine blades. 59-66 Sarkar and Voke 63 carried out an LES study of interactions of passing wakes and inflexional boundary layer over a low-pressure turbine blade and Fig. 6 shows flow structures due to the complex interactions of passing wakes and the separated shear layer. They further explained that flow topology generating coherent structures owing to the interactions of passing wakes and the separated shear layer over the blade could be schematically illustrated in Fig. 7.

4.2. LES applications in gas turbine combustors

The gas turbine has a wide variety of flow regimes from mainly high Reynolds number fully turbulent flows to transitional flows in some areas. The combination of such a wide range of flow phenomena with complex geometry makes it very difficult to model with the RANS approach. LES has demonstrated considerable promise for reliable prediction of flows in the gas turbine, especially those dominated by shear layer mixing such as in combustion chambers and exhausts where LES has demonstrated a clear superiority over RANS for moderately complex geometries. LES applications in gas turbines have been reviewed by Menzies⁶⁷ and the focus here is on LES applications in combustors.

It becomes more complicated and places additional demands on LES to simulate reacting flows since the reaction results in large changes in density and temperature and

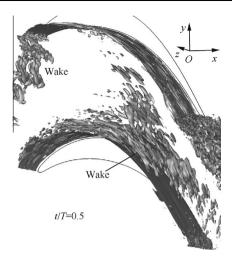


Fig. 6 Iso-surface of vorticity at an instant of time through the wake passing cycle showing flow structures.⁶³

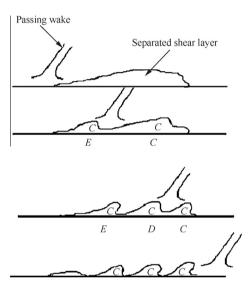


Fig. 7 Schematic of coherent vortices formation mechanism. 63

additional transport equations for the fuel distribution need to be solved. In aeronautical gas turbines, liquid fuel is used and hence the spray behaviour and its interaction with the gas phase including droplet break-up, evaporation and the interaction of the droplets with the turbulent eddies need to be captured in the simulation. In addition since combustion occurs at the very small (unresolved) scale a combustion SGS model is required to account for the two-way interaction between turbulence and combustion. Despite these additional modelling assumptions required and the complexity of the flow to be represented, LES has been applied successfully to simulating the flow in real combustion systems. A recent comprehensive review in this area is given by Gicquel et al.⁶⁸

4.2.1. Swirled fuel injector simulations

Real gas turbine fuel injector usually includes complex flow passages or veins with multiple obstacles and wing profiles that impose a rotating motion to the air streams to achieve better mixing. LES studies under iso-thermal conditions were carried

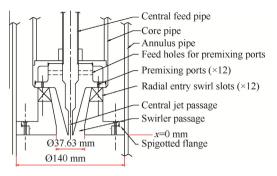


Fig. 8 Fuel injector geometry. 69,70

out to investigate the intense mixing processes between the air and fuel streams in the near field of a swirling flow fuel injector typical of some gas-turbine engine combustors.^{69,70} Fig. 8 shows the fuel injector geometry and Fig. 9 presents comparisons of the first moment (mean value) of both axial velocity $\langle \bar{U} \rangle / U_s$ and the scalar concentration $\langle \bar{\phi} \rangle$ along the radial direction (r) normalised by the outer diameter of the swirl stream D_s against experimental data, with emphasis on the near-field of the fuel injector where turbulence activity is the highest and scalar mixing the most rapid. It can be seen from Fig. 9 that the predictions are in very good agreement with the experimental data, demonstrating that the LES approach is capturing the correct physics. Further analysis of LES data provides evidence of the occurrence of the unsteady, helically spiralling vortex structures observed experimentally, and in fact identifies the origin of these as being a rotating separation event inside the fuel injector itself as shown in Fig. 10.

Due to the intense swirl of the fuel injector a recirculation region is generated, usually located immediately downstream and right along the axis of the swirled fuel injector. This recirculation is called inner recirculation zone (IRZ) (also called central recirculation zone in some literatures) and one of the main difficulty is to predict the IRZ accurately. Two swirled fuel injector flows were simulated using LES^{71,72} to assess flow dynamics and more specifically the position and breakdown of the IRZ. An LES⁷³ was performed to study comprehensively the confined swirling flows in an operational gas turbine fuel injector and the calculated mean velocities as well as turbulence properties show good agreement with experimental data.

4.2.2. Single sector simulations

Kim et al.'s LES study of a gas turbine combustor flow⁷⁴ was probably the first application of LES in a realistic gas turbine combustor (General Electric's lean premixed dry low-NO_x LM6000). The main objective of their study was to evaluate the potential of LES for design studies of realistic combustor. Their computed results agreed well with experimental data in spite of relatively coarse grid resolution employed. Their results have provided significant confidence that LES capability for design studies of practical interest is feasible in the future. More LES studies on real combustion chamber started to appear from 2004^{75–79} which mainly focused on a single sector description of the full annular gas turbine combustor thereby imposing a periodic hypothesis on the flow realisation. Although the periodic assumption would not truly represent the flow in a full annular gas turbine combustor it would reduce the computational overhead of LES significantly.

Fig. 11 shows computational domains used in a single sector LES studies.

Since it is almost impossible to measure in details the reacting flow in real gas turbine combustors while it is possible to measure velocity, temperature and species fields in a whole

laboratory combustor, real combustor data are usually limited only to a few temperature measurements at the chamber outlet and the total flow rate. One of the most important parameter that engineers would like to know is the mean exit temperature field of the combustion chamber because it controls the life-

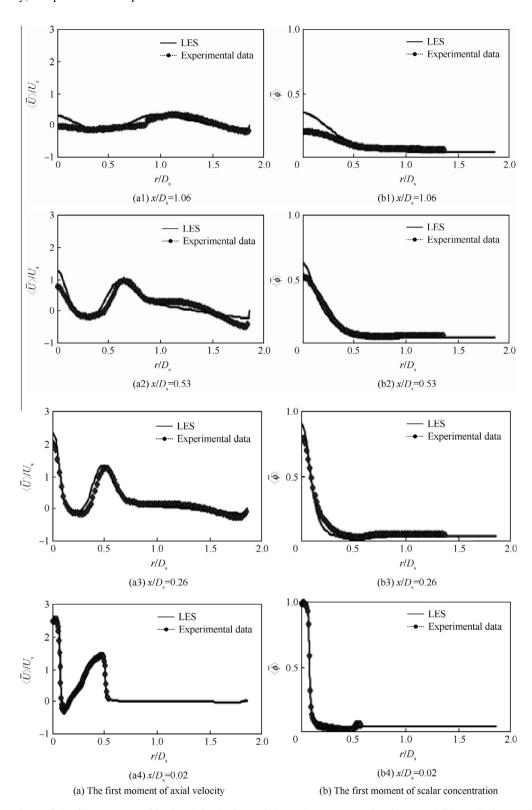


Fig. 9 Comparison of the first moment of both axial velocity and the scalar concentration between LES predictions and experimental data.⁷⁰

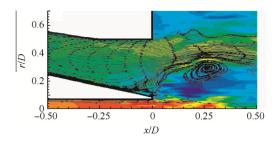


Fig. 10 Instantaneous LES predicted streakline visualisation.⁷⁰

time of the turbine blades. Fig. 12 shows the normalised temperature profiles at the outlet of different real combustors and it can be seen that LES predictions are much better than the RANS predictions when compared against experimental data.

4.2.3. Full annular burner simulations

With the increase in computing power plus the availability of thousands of CPUs or even more it is possible to perform LES of a realistic full annular gas turbine combustor, which have been done recently. 80-84 Nevertheless computationally it is very expensive and only necessary if information proceeds

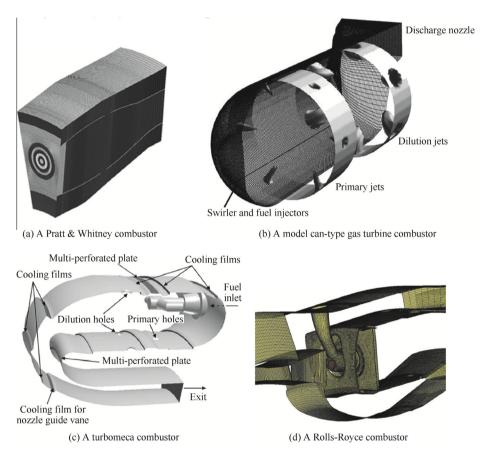


Fig. 11 Computational domains used in a single sector LES studies^{75–77}.

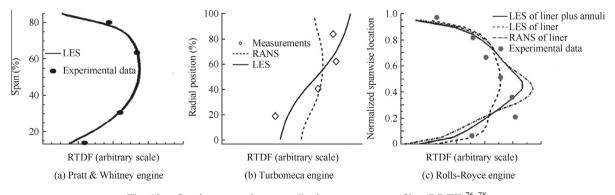


Fig. 12 Combustor outlet normalised temperature profiles $(RDTF)^{76-78}$.

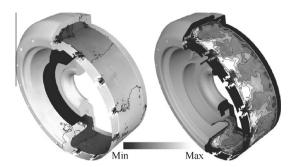


Fig. 13 Pressure iso-contours and temperature iso-contours on a cylindrical plane.⁸⁴

in the azimuthal direction which cannot be properly captured with a single sector hypothesis such as simulating flame propagation from a burner to the next after ignition and neighbouring flames that interact with each other or the existence of an azimuthal thermo-acoustic instabilities.

In the LES study of combustion instability in an annular helicopter combustion chamber equipped with 15 burners by Wolf et al. 84 three grids were used and the fine grid consists of 336 million elements. Fig. 13 shows a snapshot of the temperature field on a cylindrical plane along with the pressure field that exhibits the presence of azimuthal pressure waves. They observed that the flames oscillate azimuthally, moving from left to right at a frequency close to 750 Hz. This azimuthal motion is accompanied by an axial displacement of all flames as well, which can never be captured by a single sector LES.

These studies have shown that LES can, at least, reproduce macroscopic unsteady flow in real gas turbine combustors and the results not only provide a demonstration of the current status of LES when used on massively parallel computers but also give massive unsteady flow field information which can never be obtained by other means. Indeed such unsteady fields need now to be studied to feed the design chain and complement design assessments based on RANS.

5. Challenges/issues of LES

Despite more than half a century's intensive research/development, validation and applications in LES it has not become a mature numerical simulation tool which can be used with ease to perform complex engineering flow analysis. There are still many challenges/issues which will be discussed very briefly in this section and much more comprehensive discussion can be found elsewhere. 85-91

5.1. Development of accurate SGS models

There have been a lot of efforts made to develop new SGS models and the number of SGS models has increased significantly with numerous SGS models available now.^{2–16} Nevertheless, not many of those SGS models have been widely used (the simple Smagorinsky model and its variants are still probably the most widely used models) and hence one may argue that what is the point of developing a new SGS model? The argument is that if one takes "the traditional or proper LES approach" (more than 80% of the turbulent kinetic

energy should be resolved and hence SGS may not play an important role) for fully turbulent flows maybe there is no need to develop more accurate and complex SGS models but there are many situations where the available SGS models are inadequate such as transitional flows, relaminarization and flows where aeroacoustics, mixing and chemical reaction need to be simulated accurately. In particular, when LES is applied to practical engineering calculations (complex geometry and high Reynolds number) it is not possible in many cases for the LES mesh to resolve more than 80% of the turbulent kinetic energy, which inevitably requires a more advanced and accurate SGS model to properly model the effects of SGS motions.

5.2. Generation of inflow boundary conditions

As already discussed in more details in Section 2.3.2 that specifying inflow boundary conditions properly are crucial for LES, and yet it is an extremely difficult task to generate inlet boundary conditions accurately in LES. Intensive research has been going on in the past decades and many inflow boundary condition generation methods have been developed. 17-21 However, all those methods as discussed in Section 2.3.2 can only generate inflow turbulence with certain properties and no robust methods available yet to generate inflow turbulence with all the desired characteristics such as turbulence intensity, shear stresses, length scales, power spectrum and proper turbulent structures, i.e., coherent eddies across a range of spatial scales down to the Kolmogorov scale which interact with each other. Therefore research is still much needed in this area.

5.3. Wall layer modelling

Simulating near wall flow regions accurately is essential in many practical engineering configurations in order to correctly predict skin friction, heat transfer and so on. Ideally one needs to resolve the near wall flow structures (wallresolved LES). However, close to walls, the flow becomes dominated by vortices with a characteristic length and spacing much smaller than those of the free flow. It is well known that when Reynolds number increases the mesh resolution needs increase correspondingly in the near-wall region, this re-dependence of the resolution is much steeper, since the near-wall eddies that need to be resolved scale with wall units. In most practical engineering flows, if not all, Reynolds number is very large and it would become far too expensive to perform a wall-resolved LES. It is therefore a big challenge to model the near wall flow properly in LES as many wall models such as the much earlier near wall treatments^{25,26} by adjusting the velocity near the solid wall to enforce the local near wall flow to satisfy the logarithmic law of the wall, similar to the wall function approach used in the RANS, are not satisfactory because in many engineering flows the assumption of the existence of a logarithmic law does not hold due to the presence of strong favourable or adverse pressure gradients, separated flow regions and highly threedimensional behaviours. A comprehensive review on wall layer modelling is provided by Piomelli⁹² and as rightly pointed out by the author that "despite the increased attention to the problem, no universally accepted model has appeared".

5.4. Accurate and robust numerical methods for unstructured grid

Most engineering flows occur in complex geometries such as flows in turbomachinery and significant efforts are required to generate good quality structure grids. Hence unstructured grid methods have become much more prevalent for RANS simulations because for complicated geometries the time needed for generating unstructured grids is significantly less than that for block-structured grids. Exploration of unstructured methods for LES has increased 93-98 and the requirements for numerical schemes in LES is more stringent than in RANS since in LES it is crucial to eliminate numerical dissipation. Hence, probably the main challenge in utilising unstructured grids for LES is the difficulty in deriving higher-order (second-order or above) robust unstructured schemes that discretely conserve not only first-order quantities such as momentum, but also second-order quantities such as kinetic energy. A non-dissipative algorithm for unstructured grids was developed and applied to a variety of flows including a turbine combustor. 94,95 There are also other issues when employing unstructured grids for LES such as the effects of different grid topologies (i.e., prismatic versus tetrahedral), rapidly changing grid volumes and etc. and only limited knowledge/experiences are available.

5.5. LES for compressible flows

Much less work has been done in LES for compressible flows compared with LES for incompressible cases and there are many challenges/issues in this area. For supersonic flows with shock waves extra efforts/requirements are needed to capture the shock in a stable and accurate manner, and at the same time provide the spatial accuracy required to simulate some of the fine-scale structures inherent in turbulence. Shock waves are most commonly treated by low-order methods, often employing upwind schemes, which are not really appropriate for LES.

In compressible flows, to avoid the introduction of SGS terms in the continuity equation Favre filtering is usually adopted and hence the knowledge/experiences gained in incompressible flows may not be relevant. In addition due to extra equations such as energy equation should be solved for compressible case more SGS terms such as SGS heat flux need to be modelled, which makes SGS modelling for compressible flows much more complicated. More details on LES for compressible flows can be found in a book by Garnier et al. ³⁶

5.6. LES of turbulent combustion

LES of turbulent combustion started to appear in the 1990s and has increased very rapidly in the past decade with applications in a range of combustion problems. As chemical reactions occur on very small scales (usually smaller than the resolution of LES mesh), most of the combustion chemistry is occurring in SGS and models need to be developed. Despite this LES has shown great promises in this area and demonstrated clear superiority over the RANS approach even with relatively simple SGS combustion models. Nevertheless there are tremendous challenges in this area because turbulent combustion is so complex, e.g., in aircraft engines it involves liquid

fuel injection, liquid fuel atomization, droplets breakup and evaporation, large scale turbulent fuel air mixing, small scale molecular fuel air mixing, chemical reactions, and turbulence/chemistry interactions. Many of these processes occur on multiple time and length scales. Much more discussion on LES of turbulent combustion can be found in two review articles by Pitsch et al. ^{99,100}

5.7. LES for aeroacoustics

Noise is becoming an more and more important environmental issue and a significant proportion of noise comes from air and land transport such as jet noise, fan noise, airframe noise and high-speed train noise. There are many physical processes which can produce noise and here only aerodynamic, flow-induced noise will be discussed (aeroacoustic) and turbulence is one major source of the aerodynamics noise. Since large scale fluctuations, which are known to contribute most to the noise generated in many problems, are computed directly in LES, which makes LES a very useful tool in aeroacoustics. Applications of LES for predicting aerodynamics noise probably started in the 1990s and has become a very active research area. ^{100–115} A comprehensive review can be found in a dedicated book. ³²

LES holds great promise for aeroacoustics computations, from advancing fundamental understanding of noise generation, to improvements in source modelling for acoustic analogies and practical prediction and design of engineering systems in the near future. If properly implemented and validated, LES codes should be able to simulate the flow physics accurately that captures the transfer of energy from turbulent to acoustic modes. Nevertheless significant challenges remain from proper SGS modelling to numerical issues such as high-order accuracy and careful application of the boundary conditions, to practical engineering configurations where flow Reynolds number is usually very high and it is impractical to apply LES for both noise source capturing and its propagation. In addition, for relatively simple LES applications, conventional validation analysis may be performed against accepted experimental databases (first order and second order quantities). For LES applications in aeroacoustics extra care should be taken for proper validation as shown in aeroacoustics theory that complicated statistics such as two-point space-time correlations are critical to flow-generated sound. Hence the validation, perhaps, can start with the simplest statistics and progressing to the more complex and acoustically relevant statistics.

6. Concluding remarks

This paper describes briefly LES formalism first followed by a short introduction to the history of LES and its development and a review of LES applications in transitional flows and gas turbine combustor flows. Several major challenges/issues associated with LES and its application such as SGS modelling, generation methods for inflow boundary conditions, wall layer modelling, LES of turbulent combustion etc. have also been briefly discussed.

Since the 1960s researches have obtained great advances in the field of LES with demonstration of its capabilities in calculations of complex turbulent flows and its superiority over

RANS in numerous cases. Nowadays, thanks to the rapid progress of information analysis systems and various simulation codes, LES has become a very powerful and popular tool in simulating turbulent flow, and has been widely used for not only turbulent flow analysis but also for combustion, aero-acoustics and many other areas. It has also been demonstrated that it is feasible to perform LES of complex engineering flows such as a realistic full annular gas turbine combustor.

With its huge amounts of flow information included in 3D unsteady flow field, LES will be undoubtedly the main tool for engineering fluid analysis within a couple of decades since DNS will still be far too expensive. In the future, LES is likely to become used for a broader range of flow problems and for more complex problems including more multi-disciplinary applications. Nevertheless, there are still significant challenges remaining as discussed in this paper before LES can become a reliable, robust engineering analysis tool which can be used as an alternative to RANS. For the foreseeable future it is very unlikely that LES will replace RANS completely and become a design tool used by design engineers without extensive years of LES experiences.

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