

Large Eddy Simulation

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ABSTRACT

Large eddy simulation (LES) is an emerging technique for obtaining an approximation to turbulent flow fields. It is an improvement over the widely prevalent practice of obtaining means of turbulent flows when the flow has large scale, low frequency, unsteadiness. An introduction to the method, its general formulation, and the more common modelling for flows without reaction, is discussed. Some attempts at extension to flows with combustion have been made. Examples from present work for flows with and without combustion are given. The final example of the LES of the combustor of a helicopter engine illustrates the state-of-the-art in application of the technique.

Keywords: Computational fluid dynamics, large eddy simulation, turbulent flow, subgrid modelling, dynamics smagorinsky model, approximate deconvolution model

1. INTRODUCTION

It is now a common practice to conduct analyses of devices or vehicles or even natural phenomena like the weather by solving partial differential equations that describe flows. While formulas and empirical relations remain useful, computational fluid dynamics (CFD) has become a tool of choice. The methods for numerical solution of differential equations are now understood well, and computers are powerful enough, that CFD solutions of laminar flows are generally quite reliable. Turbulent flows present a lasting difficulty: These flows contain a wide range of scales of motion, and therefore a wide range of length and time scales, that a direct computation of most flows encountered in practice is not feasible, and perhaps not necessary. In many cases, it would be sufficient to know the fields of mean quantities such as the mean velocity, but even the computation of mean fields, termed RANS for the Reynolds-averaged Navier-Stokes equations that are solved, is not as reliably accurate in general because the equations are nonlinear. Models are needed for some terms in the equations for the means, and it is widely understood that the demands on such modelling are too severe. Nevertheless, it is possible to use CFD solutions in such cases also by restricting predictions to classes of flows for which the accuracy of the modelling has been determined. In this article, a different technique for computing a different approximation of turbulent flows in which the requirements on the modelling are comparatively less but at increased computation cost is discussed. This trade-off is not the only benefit as will be seen below in the article. The technique is called large eddy simulation (LES).

An LES is a computation of a large-scale part of a

turbulent flow. If the equations had been linear, this would have been straightforward. Instead, any approximation like LES results in unclosed terms which must be modelled. The main expectation is that the dynamics of a range of large-scales will be obtained accurately, and that this is sufficient to obtain close estimates of several quantities of interest, with better accuracy and reliability than a RANS solution. The basis is that most of the kinetic energy in a turbulent flow is accounted for by the large-scale motions, that the flow generally interacts with its boundaries on large-scales, and that small-scale dynamics is nearly universal. Differences in flows arise from the different boundary and initial conditions; when these are, for example, the different bodies embedded in a flow, an LES accounts for the interaction of the flow with these objects. If small-scale motions have universal behaviour, it should be easier to find general models than in RANS computations which require modelling of both large- and small-scale dynamics. In fact, even though a model is a formal requirement for an LES, since the model is for the effect of small-scale motion on the computed large-scales, when this effect is small the solution may not be sensitive to the model. This has been the general experience, but is often viewed with surprise because RANS solutions have been notoriously sensitive to its turbulence models. In LES, models that appear to be poor in *a priori* tests (tests of the model using exact flow fields at some instant) have given acceptable results in simulations. Simulations without explicit LES models have also given acceptable results and are now termed implicit LES (ILES) denoting a modelling for LES provided by the numerical scheme.

An LES is a newer type of computation of a turbulent

flow that seeks to overcome the deficiencies of RANS by deploying more computer resources. The basis for RANS is quite sound for many flows. Consider a turbulent flow of water through a long pipe under a constant (stationary) head. Although the velocity at any point, or the mass flux through any cross-section, will exhibit significant fluctuations in time, we would find much smaller variations in the amount of water collected during equal finite intervals, as long as the intervals are not too small. In other words, one expects turbulent flows to have means. The flow at any point in the pipe is also stationary and a mean velocity field can be found that varies slowly along the pipe, more rapidly over a cross-section, and most rapidly near the pipe wall. Such flows are obtained quite accurately with a RANS computation because the turbulence changes little from place to place in the flow.

Now consider a small object placed in the pipe. Generally, there will be some kind of intermittent shedding into the wake of the object. All flow quantities in the vicinity of the object will acquire variations in time corresponding to the time scale of the shedding process. There are associated length scales of the order of the size of the object. Now, a RANS solution becomes more difficult. Although one may still expect means to exist, the fluctuations contain large-scale unsteadiness. RANS modelling, which accounts for the enhanced transport by turbulent fluctuations, must now account for the effects of large-scale unsteadiness. If an accurate description of the near wake is needed, LES becomes a good choice because it naturally captures the large-scale unsteadiness.

Initially as CFD tools were deployed for analyses, it was encouraging that reasonable answers were obtained for flows in complex geometry. Even when there was a significant difference between an experiment and a RANS solution, and by different amounts in different parts of the flow, such solutions were still useful indicators of how the solution would change when some input parameters were varied. However, if we seek to design the flow for significant performance improvements, an LES becomes necessary. An LES can be used to guide local changes better, such as placement of injectors, or even the continuous variations that a formal shape optimisation algorithm might give. It is then a tool for more demanding applications that can accommodate the increased computing costs.

For readers who would like to pursue LES in their work, the necessary background on turbulent flows can be found in Pope¹⁸. An early review was provided by Lesieur and Metais¹². Pitsch¹⁵ writes on developments in LES for reacting flows. A textbook for LES, covering a broad range of topics in LES, is by Sagaut²⁰ and includes an extensive bibliography. A conference series called Direct & Large Eddy Simulation (DLES) has been organized every two years since 1994

2. DEFINING AN LLARGE EDDY SIMULATION PROBLEM

Some essential aspects of an LES can be understood

by considering the simpler problem of a one-dimensional transport equation. Let the function $u(x, t)$ satisfy the transport equation

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \quad (1)$$

The problem specification is completed by adding initial and boundary conditions on u . Suppose we wish to find an approximation $U(x, t) = G*u$ rather than u itself (convolution operator G will be defined below). Formally, the governing equation for U can be obtained by applying the operator G to Eqn. (1) to get

$$\frac{\partial U}{\partial t} + G* \frac{\partial f(u)}{\partial x} = 0, \quad U = G*u. \quad (2)$$

For completeness, we would apply the same operator to initial and boundary conditions. The problem defined by Eqn. (2) would be equivalent to that defined by Eqn. (1) if it were possible to invert the operation on u . In an LES, G is a low-pass filter and U is a large-scale part of u . In RANS, G is a time-averaging or an ensemble averaging operator. It is obvious that one cannot recover the signal from its average alone (G as an averaging operator is not invertible). In an LES, G as a low-pass filter discards information on scales smaller than some cut-off and is also not invertible. So, the problem defined by Eqn. (2) is not equivalent to that of Eqn. (1) for operators G of our interest.

They can re-write Eqn. (2) as

$$\frac{\partial U}{\partial t} + \frac{\partial f(U)}{\partial x} = R(u, U), \quad (3)$$

where the RHS of Eqn. (3) ,

$$R(u, U) = \frac{\partial f(U)}{\partial x} - G* \frac{\partial f(u)}{\partial x}, \quad (4)$$

vanishes if $f(u)$ is a linear function of u . Then, problem in Eqn. (3) is closed, and it does not matter that u cannot be recovered from U . When $f(u)$ is nonlinear, it is necessary to find a model for $R(u, U)$, since it contains a quantity, u , which cannot be obtained from U . Closure requires that they have a model $R_m(U)$ in terms of the computed quantity U . In RANS of incompressible flow, this term arises due to the nonlinear convection terms in the momentum equations and is called the Reynolds stress. The RANS problem is closed by providing a turbulence model. In LES, such terms arising from the same convection terms are called sub-grid stresses and closure is obtained by sub-grid modelling.

So the LES problem is defined by applying a low-pass filter to all the equations defining the original physical problem (both differential equations and initial/boundary conditions) and prescribing a sub-grid model. Although much effort has gone into investigating different sub-grid models, there have been other requirements which are unique to LES, such as time-accurate numerical schemes, and prescribing fluctuating, turbulent, inflow boundary

conditions. Also, most LESs have been formulated where the low-pass filter is spatial but temporal filtering has also been investigated. Owing to the implied dispersion relations, small-scale motions are related to small periods or high frequencies. A low-wavenumber-pass filter will also filter out dynamics of high frequency motions and similarly, a temporal filtering out of high frequency components will filter out large wavenumber (small-scale) motions.

2.1 Sub-grid Modelling

Early computations, that have been termed LES, were those that were clearly on too small a grid to resolve much of the turbulent scales. It was to compute atmospheric flows which had very large Reynolds numbers and consequently, a very large range of scales. A term was added to the momentum equation, similar to the eddy viscosity term used in RANS. The eddy viscosity for RANS takes a length scale which is an estimate of the integral scale of the turbulent flow, and a velocity scale which is of the order of the velocity fluctuations. The analogous model for LES is known as the Smagorinsky model¹⁷, the length scale is a mean-grid spacing and the velocity scale is obtained from the local velocity gradient. In LES, the model is for the effect of uncomputed small-scales on the computed large-scales. The uncomputed scales are then of the order of the grid spacing, and smaller, so that the model is commonly termed a sub-grid-scale (sgs) model.

The simplest turbulent flow is an incompressible flow of a Newtonian fluid. The governing equations are the Navier-Stokes equations for a divergence-free velocity field \mathbf{u} :

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0.$$

On applying a low-pass filter we get the equations

$$\rho \left(\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U} \cdot \nabla) \mathbf{U} \right) = -\nabla P + \mu \nabla^2 \mathbf{U} + \left((\mathbf{U} \cdot \nabla) \mathbf{U} - \overline{(\mathbf{u} \cdot \nabla) \mathbf{u}} \right), \tag{5}$$

$$\nabla \cdot \mathbf{U} = 0 \tag{6}$$

for the uppercase variables, which are the low-pass filtered velocity and pressure fields, (line over variables or terms denote low-pass filtering). Note that there is no term involving \mathbf{u} in Eqn.(6) because it is a linear equation. The last two terms on the RHS of Eqn. (5) can also be cast in the form of the divergence of a tensor $\tau = \mathbf{U}\mathbf{U} - \overline{\mathbf{u}\mathbf{u}}$ termed the sub-grid stress tensor (a stress because they appear in the momentum equation). The simplest model is to take this stress to be proportional to the large-scale strain rate $\varepsilon(\mathbf{U})$ with an eddy viscosity coefficient ν_s to be obtained by calibration as in RANS. Then $\tau = \rho \nu_s \varepsilon$, and for the Smagorinsky model

$$\nu_s \propto \Delta^\gamma \|\varepsilon\| \tag{7}$$

What does this model achieve? When inserted into

the momentum Eqn.(5), the effective viscosity in the flow is the sum of the eddy and the molecular viscosity. Where velocity gradients are large, this term acts to reduce the magnitude of the gradient. The eddy viscosity itself is more effective where the velocity gradients are large, but diminishes as the grid spacing is reduced. For further understanding, consider the general spectral dynamics in a turbulent flow. Turbulent flows interact with their boundaries on the scales of the bounding surfaces (chord and span of a wing, pipe diameter, radius of curvature of a pipe bend, etc.) and the motions on these scales interact, generating smaller scales in a cascade with little dissipation of kinetic energy. The cascade is cutoff at small-scales when the velocity gradients are large enough for dissipation to become dominant. In an LES, the smallest computed motions are still much larger than the dissipation scales. So the transfer of energy is disrupted. If this transfer of energy is prevented, energy builds up at the computed small-scales and the solution becomes unbounded. In mathematics, this calls for a regularisation of the approximate problem (the LES problem) because the divergence or appearance of a singularity is due to the approximation. The complete problem, which includes all relevant small-scales, does not have this singularity (often accepted, but without a proof).

The role of the LES model is to allow the transfer of energy from the computed large-scale motions to uncomputed small-scales. An eddy viscosity model dissipates kinetic energy over that due to the physical process implied by the molecular viscosity. The effect increases with wavenumber. A calibration constant such as C_s can provide an adequate amount of dissipation. When this constant is larger than necessary, the computation will be stable but inaccurate; when it is too small, the inadequate dissipation will cause the solution to diverge. We may easily accept some error in the dynamics of the smallest computed scales, but with a simple model like the Smagorinsky model, we must accept that there is some error in the dynamics of the large-scales also.

2.2 Initial and Boundary Conditions

Prescribing initial conditions for an LES problem does not present any special difficulty. The required solution is unsteady but stationary, and effects of initial conditions are expected to have disappeared when statistics are taken. Boundary conditions, on the other hand, require special attention. In some simulations, the conditions at inflow boundaries are laminar, and transition to turbulence occurs within the computational domain. Then, either steady or unsteady, deterministic or stochastic, inflow conditions may be specified. If the inflow is turbulent, the inflow conditions need to be the unsteady field of a relevant turbulent flow over the inflow surface. If, instead, some kind of stochastic field is supplied, since the correlations among the fluctuations are not those of a turbulent flow, these fluctuations will decay until regenerated with correct correlations in downstream shear layers. This inflow length can add significantly to the computational domain size.

Another approach has been to perform a precursor simulation (LES) of a closely-related turbulent flow and supply the solution from a plane as the inflow boundary condition. For example, when simulating a turbulent boundary layer responding to changing geometry, pressure gradient, protrusions, etc., the inflow condition can be taken from an LES of a flat plate turbulent boundary layer of the required thicknesses. A more economical approach is to take the downstream boundary layer, rescale it to the thickness required at inflow, and use it as the condition at the inflow. Outflow and far-field conditions can be prescribed as would be appropriate even for laminar flows, such as fully developed, non-reflecting, or convective conditions.

3. STANDARD SUB-GRID MODELS

Sub-grid models may be broadly divided into functional and structural models. A functional model provides expected properties of the model and the Smagorinsky model and dynamics Smagorinsky model are examples. These models provide dissipation as a model for the transfer of energy to small-scales. The second kind is a structural model. Here, an estimate of the full field including the sub-grid scales is found and the sgs stress is calculated.

3.1 Smagorinsky Model

The Smagorinsky model is

$$\nu_s = (C_s \Delta)^2 \left(2 |\bar{S}^2| \right)^{1/2}$$

with the value of the coefficient C_s often adjusted to obtain the best results. Typical values for shear flows are 0.1 to 0.12. This model is still in wide use, perhaps because it is simple to implement and will at least stabilise a computation.

3.2 Dynamic Smagorinsky Model

A dynamic model is a procedure that finds coefficients such as C_s from the simulation field itself, during the course of the simulation such that some expectation is met. This idea was first proposed in conjunction with the Smagorinsky model for the eddy viscosity by Germano¹⁹, *et al.* The principle used was that the sgs stress should have the same form with the same coefficient even when the small-scale cutoff size is changed. In practice, one field is obtained with the given grid, and the second is obtained by filtering the solution to a grid whose spacing is twice that of the original. This procedure returns a Smagorinsky coefficient which evolves with the flow and varies in space. Sometimes the value so obtained can be negative. Either a limit, and/or averaging over homogeneous directions is done to maintain a positive dissipation. The success of the dynamic Smagorinsky model has been a turning point for LES taking it from a subject for research to applications.

3.3 Scale Similarity Model

Bardina¹, *et al.* modeled the sgs stress $\tau = UU - u\bar{u}$ as $\tau_m = \bar{U}\bar{U} - \bar{U}\bar{U}$. The field \bar{U} is obtained by filtering the LES solution at every time step. The expectation is that

the stress, which is due to nonlinear terms containing the sub-grid part, should be represented adequately by applying a filter to the LES field itself. While this estimate of the sgs stress shows good correlation with the actual sgs stress in *a priori* assessments with DNS data, in actual computations, this model does not provide an adequate dissipation.

3.4 Chollet-Lesieur Spectral Model

These models originate from an analytical theory of turbulence⁵. An effective spectral viscosity function $n_\epsilon(k/k_c)$, which is a function of the wavenumber k scaled with the cutoff wavenumber k_c , is used to model the energy transfer rate. This viscosity rises sharply near cutoff. There is an extension to a physical space model also.

3.5 Mixed Model

A mixed model combines one the many models devised to have a closer correlation to the sgs stress, such as the scale similarity model, or tensor diffusivity model, etc., and adds a term proportional to the Smagorinsky model term which provides an over-riding dissipation.

3.6 Deconvolution

The approximate deconvolution model (ADM)¹⁶ drew wide attention because of the significantly better results that were reported. Both ADM and the several versions of the velocity estimation models⁸ were procedures to estimate a flow field with small-scales beyond that of the LES field and use this estimate to construct the sgs stress. By approximate deconvolution of the LES field U , a field u^* was found as an estimate for u . In velocity estimation models, there were sub-steps in the LES computations on a grid of twice the size, this extending the small-scales to twice the wavenumber, to obtain the field u^* which has this additional small-scale content. Similarities between these two developments have been discussed in a joint paper⁷ by the principal authors of two methods.

3.7 Explicit Filtering

The explicit filtering approach of Mathew¹³, *et al.* follows from the observation that the ADM procedure can be reduced to an integration of the discretised, unfiltered equations of the problem with a low-pass filtering of the primary fields, say velocity, density and temperature or enthalpy after time step. It is necessary that the spatial operations such as differentiation, interpolation, etc., be performed with high-resolution schemes that are accurate over most of the represented length scales; also, the low-pass filter should not filter out a large part of the represented large-scales. It was shown that such an approach provides an adequate LES model without adding any model terms to the problem equations.

The explicit filtering method combines features of several of the models listed above. Filtering is effectively like the Smagorinsky dissipation, except that it is weighted towards high wavenumbers. Scale similarity model is implicit,

though it is more easily understood in the ADM formulation. The shape of the explicit filter provides an effective spectral viscosity, which is like that of the Chollet-Lesieur special model.

3.8 Implicit Large Eddy Simulation

Several computations without any explicit model terms or procedures for LES modelling were found to be suitable for LES. The earliest example was the use of the Boris-Book scheme devised for shock capturing. Since the result of turbulence simulations on a grid, that is too coarse to capture the small-scale dynamics, is the appearance of wiggles, just as in flows with shocks, a method that suppresses these wiggles is effective for LES also. The ILES of Visbal and Rizzetta¹⁹ was initially devised to obtain stable solutions with high-resolution compact difference schemes by high-order filtering. In effect their scheme meets all the requirements of the explicit filtering method listed in section 3.7. For LES of aeroacoustics, Bogey & Bailley³ also use the explicit filtering approach (they called it selective filtering) coupled with very high-order difference schemes, motivated by the requirements of aeroacoustics LES.

4. LARGE EDDY SIMULATION FOR REACTING FLOWS

Methods for LES of combustion are not yet well-established. Combustion, rather than reacting flows in general, presents a conceptual difficulty. LES of non-reacting flows are based on the expectation that the flow interacts with its surroundings on large-scales, that most of the energy is contained in large-scales, and that the dynamics of small-scales do not alter the evolution of the large-scales except to the extent that the dissipation at small-scales drain the energy cascading from the large-scales at a certain rate. The large-scale dynamics would be altered if this energy transfer rate is not obtained in the simulations.

In turbulent combustion, on the other hand, there is an essential process that occurs only at small-scales; in typical examples of technical combustion such as in engines, reaction rates are high enough that flames are very thin, much thinner than the smallest scales we expect to compute in LES. No part of the processes which occur in flames is computed in a typical LES. So, an auxiliary model of the effect of these small-scale processes must be provided. In combustion, the issue of flame modelling is similar for LES and RANS in that it arises from the strongly nonlinear form of the reaction rate term; an estimate of the reaction rate using the computed field can bear little connection to the appropriate source term (mean or large-scale part of the reaction rate). For RANS, the reaction rate is estimated from mixing rates or from pdf models, or CMC modelling.

Analogous approaches, and some original ones, have been studied for LES by a few groups with varying degrees of success. A common finding is that, generally, the LES provides a better prediction than a RANS for combustion.

The probable reason is that in both RANS and LES, the reaction yield is dependent on the mixing rate (species for non-premixed flames, heat for premixed flames) which can be obtained more accurately in LES. The difficulty is not so much that the flame sheet is thin, much thinner than the grid spacing, but that small-scale motions wrinkle the flame sheet and provide a much higher flame sheet area than a smooth surface over a similar region in space. Since these small-scales are not computed in an LES, this wrinkling is not obtained.

4.1 LES Models for Combustion

We consider models for non-premixed combustion first. Since the flames of interest are thin, the flame brush can be modelled as a collection of flamelets. In this limit, in the neighbourhood of every flamelet, the distribution of each scalar is obtained from the steady flamelet equations

$$\frac{1}{2} \rho \chi \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i = 0 \quad (8)$$

Here, the production rates $\dot{\omega}_i$ are a function of mass fractions Y_i and the temperature. For a given value of the scalar dissipation rate χ Eqn. (8) can be solved and a table of scalars as a function of χ and mixture fraction Z prepared before the LES. During the LES, scalars are found from the table, and then the density, which is used to integrate the LES equations for mass and momentum conservation, and transport of mixture fraction. An estimate of χ is obtained from the mixture fraction variance, or from a presumed-shape pdf which also requires the mixture fraction mean and variance as inputs. Unsteady flamelet equations have also been investigated.

A modification of the flamelet approach is the flamelet-progress variable (FPV) method, which takes mixture fraction and a progress variable during the course of the LES to look-up scalars from tables. Since the progress of the combustion is obtained from a transport equation for the progress variable (a sum of concentrations), the local state of the flame is made determinate; when χ is used, a 'burning' solution is always found in the moderately high χ hysteresis (multiple-valued) regions. So the FPV approach is an improvement for flames with local extinctions/ignitions.

An extension of the successful pdf methods for RANS is the filtered mass density function (FMDF) method for LES^{6,11}. The FMDF is a density weighted, spatial large-scale distribution function. As in the pdf method, the transport equation for the FMDF contains the reaction rate term in closed form so that, formally, no modelling of this term is required. However, other problems such as the treatment of mixing, and the increase in dimensionality do appear. Mixing models have been proposed, and a Monte Carlo approach of solving a stochastically equivalent problem provides some relief from the increased dimensionality.

There is even less experience of LES of premixed combustion. Several attempts have made using flamelet

methods with a progress variable. As in RANS, the reaction rate is obtained using models for the flame surface density.

5. APPLICATIONS OF LARGE EDDY SIMULATION

Methods for LES were assessed using by *a priori* and *a posteriori* tests. *A priori* tests refer to tests of SGS models using DNS data. The terms in the LES equations, which require a model, can be calculated from the DNS data and the accuracy of the estimation of such terms by the SGS model can be determined. Canonical flows used for such tests were homogeneous, isotropic decaying or stationary (forced) turbulence, which has spatial periodicity in a cube, or channel flows with periodicity in the streamwise and spanwise coordinates. *A posteriori* tests are assessments of the results of LES against DNS or experiments.

Often the DNS data are first filtered to the same scale range as the LES, but there is no particular merit to this approach since the objective of the LES is to obtain an approximation of the flow. It is more helpful to know the extent of the error in the approximation (LES) than how close the LES is to the DNS data, which contains only the same range of large-scales. *A posteriori* tests are available for the periodic flows mentioned above as well as for several spatially developing flows such as mixing layers, jets, boundary layers and channel flows. Many examples are available in the literature^{12,15}. Here, a few examples from their work are given.

5.1 Non-reacting Canonical Flows

As an example of LES of a non-reacting flow, consider the round jet. Well-known benchmark experiments^{12,14} at a Reynolds number (Re) of 11,000 based on the mean velocity U and jet diameter D at exit, and of Hussein¹⁰, *et al.* at Reynolds number of 95,500. These two flows were simulated with 256 x 160 and 320 x 192 gridpoints over 40 D x 10 D and 40 D x 12 D in the axial and radial directions at Re = 11,000 and 95,500, respectively. Figure 1 shows a visualisation of the jet with vorticity magnitude at the higher Re.

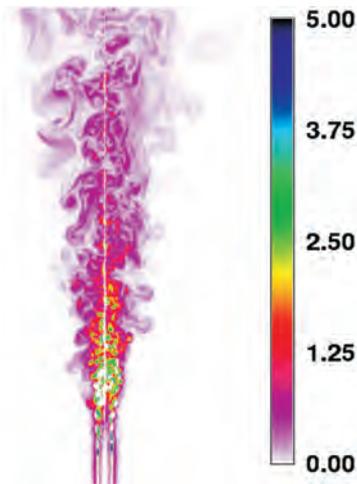


Figure 1. Round jet at Re = 95,500; vorticity magnitude contours on longitudinal section.

Figure 2 shows the decay of the centreline velocity and radial distribution of shear stress to demonstrate the quality of the LES possible. The decay constant (reciprocal of the slope from Fig. 2(a) is 5.98, as whole that in the two experiments were 6.02 and 5.8. This solution is from a recent LES using the explicit filtering approach. Results

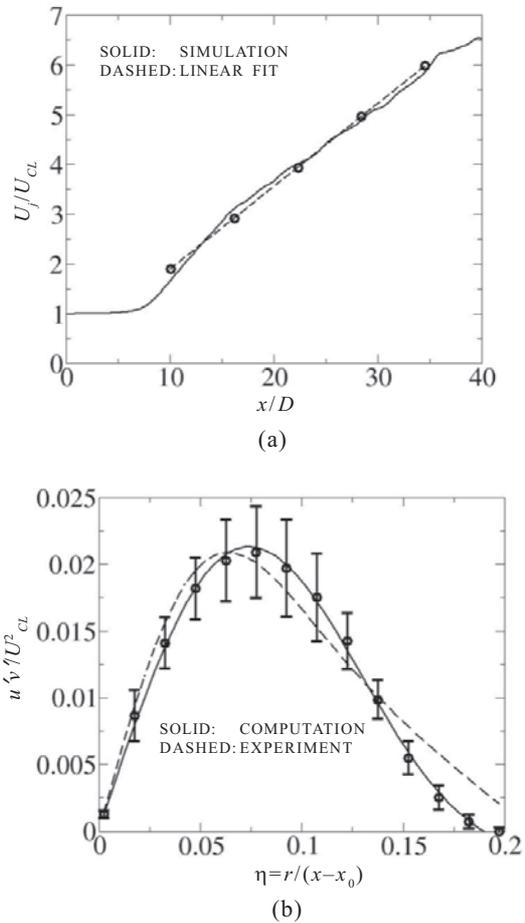


Figure 2. Round jet at Re = 95,500: (a) decay of mean velocity along centreline; (b) Reynolds shear stress in similarity variable η, error bar shows variations at different x-stations.

of earlier simulations of round jets do not show the fast breakdown at the end of the potential core followed by a clear linear growth in the reciprocal of centreline velocity. Excellent results for the same round jet experiment were reported by Bogey & Bailley³ also. Their method is also an explicit filtering approach, though it has been termed selective filtering. They use high-order finite difference schemes with large stencils and filters out a narrow range of high wavenumbers.

5.2 Reacting Canonical Flows

A few well-documented experiments have become benchmarks for assessing turbulent combustion simulations. The SANDIA flames A, B, C, D, E, F, are partially premixed, round, methane-air jets surrounded by a hot pilot co-flow, at increasing jet flow velocities. As the flow speed increases there is more local extinction. Flame A is formed

in a laminar jet, while D is a turbulent jet at $Re = 22,400$ with mild extinction. There have been several LES of flame D and some of flames E and F¹⁵.

Our initial simulations with the explicit filtering method have been a mixed success. Although the mixture fraction is predicted well, both along and across the jet, the radial profiles of temperature and concentrations showed significant differences that can be traced to excessive reaction rates. One reason for the discrepancy is that only a single-step reaction model has been used, which calls for a judicious selection of reaction rate parameters. Improvements have been observed in subsequent simulations. Figure 3 gives an impression of the flame close to the nozzle exit. Temperature contours are shown with a range of colours and the instantaneous, stoichiometric mixture fraction contour is superposed as a black curve.

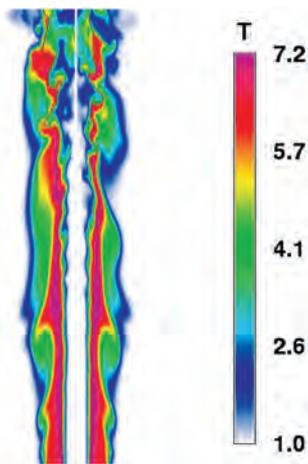
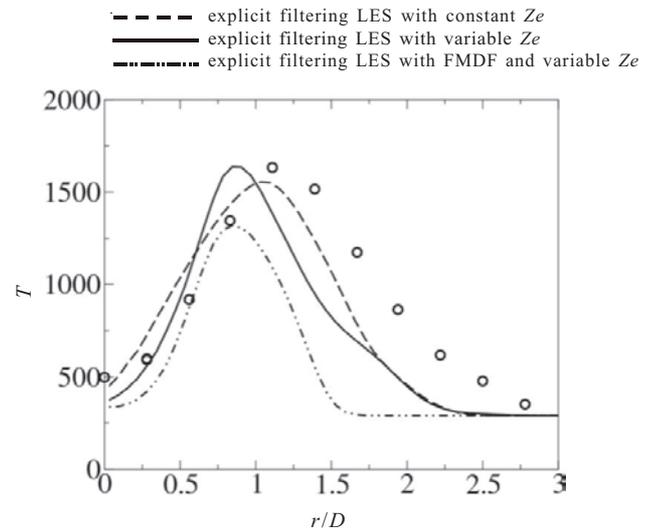


Figure 3. Contours of temperature T at an instant of SANDIA flame D, and mixture fraction contour at stoichiometric level superposed as a black curve.

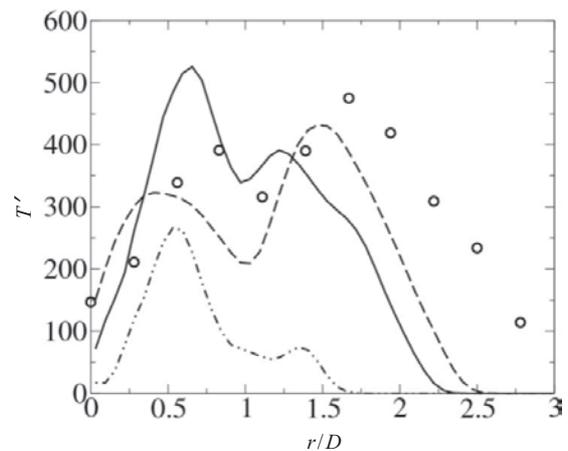
Figure 4 compares radial distributions of temperature and its fluctuations at 15 diameters with data from the experiment. Two curves are from simulations with explicit filtering LES and a WENO scheme (also a filtering scheme) for scalar transport equations. The third uses the FMDF method for obtaining the scalars. It is difficult to draw definitive conclusions at this stage. However, note that the temperature fluctuations are quite large which underscores the need for the special modelling of turbulence (an LES approach) and the reaction rate term. The pure filtering approach seems to do about as well as the FMDF in this case. The prediction of peak levels and especially the jet core region may be considered acceptable. The most notable difference is that the computed flame is narrower than that of the experiment. The solution at 7.5 diameters (not shown here) follows the experiment more closely.

5.3 Industrial Flows

Large eddy simulation are beginning to be used for industrial analyses, especially as it becomes a feature in commercial codes. For industrial applications, the search



(a)



(b)

Figure 4. Radial distributions of: (a) temperature, and (b) rms of its fluctuations.

is on for related methods such as detached eddy simulation (DES) and its variants, and hybrid RANS-LES method. The hybrid method becomes necessary because LES of wall-bounded flows have unusually large grid point requirements in the wall-normal direction. It would be easier to use a RANS solution in attached boundary layer regions, that blend into LES solution, where there is massive separation and low frequency unsteadiness.

An example of reacting flow LES is that of a combustion chamber of a helicopter engine⁹. The computation is of 36° of an annular combustion chamber designed by Turbomeca. An unstructured grid of 286,500 nodes and 1,550,000 tetrahedral elements was used. The flame was resolved in the LES by artificial thickening. RANS was also performed with 150,000 nodes and 825,000 tetrahedra. It was concluded that the LES results were more useful, in providing insight into prevalent combustion regimes (e.g., very few regions of flames at very rich conditions), as well as being closer to available experimental data (radial temperature profiles, whose non-uniformity is an important design parameter).

6. CONCLUSIONS

Large eddy simulations is emerging as a technique for engineering analyses and design as we seek to improve performance of current devices, or find new designs for more challenging applications. It is but the next step from using empirical relations or analytical results for simple flows, to CFD of laminar and simple turbulent flows, to LES. Clearly the extra effort is justified only when the detailed flow field is of interest and not merely overall balances. LES is called for when large-scale, low-frequency unsteadiness of the flow field is of interest. Over the past decade, the efforts have resulted in establishing LES practice for cold flows. Practitioners have their own favourite models and approaches which give roughly similar results. Because these results are significant improvements on RANS, LES is beginning to be used for many practical flows. LES of combustion is not as well established as RANS, but the results of attempts have been generally encouraging. A turning point for combustion LES, similar to that brought about by the dynamic Smagorinsky model, is awaited.

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