A Review of Progress on Direct and Large-Eddy Simulation of Turbulence

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Abstract

A review is given of direct and large-eddy simulation which is intended to summarise state-of-the-art research presented during the 1999 Isaac Newton Institute Programme on Turbulence. Introductions to the techniques are given, along with examples of applications across a range of turbulent and transitional flow problems. Recent developments in techniques for large-eddy simulation are highlighted. The discussion includes a summary of the guidelines proposed during the programme for practical large-eddy simulations and comments on problem areas that require further research.

1 Background

A 6-month Programme on Turbulence took place at the Isaac Newton Institute in Cambridge during the first 6 months of 1999. The programme gathered together researchers from around the world and stimulated use their complementary expertise to study aspects of turbulence in fluid flow. At any one time up to 20 academics occupied office space in the Institute building and this number was supplemented by numerous short stay participants. The programme involved participation from a core of industry sponsors (British Aerospace, Rolls-Royce, British Energy, DERA, BG Technology and the Meteorological Office), coordinated by the Royal Academy of Engineering. During the 6-month programme a number of small Workshops and larger Symposia were organised to treat specialised areas of turbulence research.

One significant area of activity during the programme concerned numerical simulation of time-dependent turbulent flow, either by direct numerical simulation (DNS) or large-eddy simulation (LES). Introductions to these areas were given during the Instructional Conference (April 6-16th), lecture notes from which will appear in [1]. More detailed discussions on LES followed during the

Mathematics of Closure Workshop (April 19-30th) and there was a large 3-day Symposium on DNS and LES, organised in collaboration with ERCOFTAC with close to 100 participants (May 12-14th), proceedings from which will appear in [2]. The Symposium consisted of 6 invited talks, 30 contributed papers and 15 poster presentations. Resident participants with interests in DNS and LES included Jim Brasseur (Penn State, 6 months), Paul Durbin (Stanford, 1 month), Massimo Germano (Turin, 1 week), Bernard Geurts (Twente, 4 months), Darryl Holm (Los Alamos, 1 month), Javier Jiménez (Madrid, 1 month), Bill Jones (Imperial, 1 month), Bob Kerr (NCAR, 1 month), Shigeo Kida (Nagoya, 3 months), John Kim (UCLA, 2 weeks), Leonhard Kleiser (ETH Zürich, 1 week), Chuck Leith (LLNL, 3 months), Tony Leonard (CalTech, 4 months), Marcel Lesieur (Grenoble, 3 weeks), Parviz Moin (Stanford, 1 week), Koji Ohkitani (Kyoto, 6 months), Wolfgang Rodi (Karlsruhe, 2 months), Neil Sandham (Southampton, 6 months), Sutanu Sarkar (UCSD, 1 month), David Thomson (Met. Office, 2 months) and Peter Voke (Surrey, 1 week). Additionally there were regular seminars and three 'industry days' where research relating to industrial applications was presented. This report is intended to bring together at least some of this activity and present it in a form accessible to a wider audience besides the participants in the programme. It will hopefully serve as a snapshot of the status of DNS and LES in the middle of 1999 and reflect some of the detailed discussions that took place about limitations of techniques and areas in need of further research. It necessarily reflects the author's own perspective and is not to be taken as a consensus of views of the programme participants.

The Isaac Newton Institute programme involved many discussion sessions, both structured and informal. In this paper a citation of a name followed by the words 'INI discussion' implies that comments were made informally in a group discussion.

2 Direct numerical simulations of turbulence

Direct simulation of turbulence is increasing in realism (complexity and Reynolds number) as computers increase in performance. Simulation databases have already been used for over a decade for fundamental research into turbulent flow, especially at the NASA-Stanford Center for Turbulence Research. A recent review is by Moin & Mahesh [3]. Here we give a brief introduction and review the range of applications now feasible.

We restrict the discussion primarily to incompressible flow for which the governing equations are

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{2}$$

2.1 Turbulence scales and resolution requirements

Turbulence in fluids is a nonlinear phenomenon with a wide range of spatial and temporal scales. Estimates for the smallest scales are available from the Kolmogorov microscales, obtained from dimensional analysis assuming dependence only upon viscosity ν and dissipation rate ϵ. The length microscale is

$$\eta = \left(\frac{\nu^3}{\epsilon}\right)^{1/4}. \tag{3}$$

If the length and velocity macroscales of the problem are l and u and if we assume dissipation scales in the same way as production, i.e. as u^3/l, we have

$$\frac{l}{\eta} = Re_l^{3/4}, \tag{4}$$

where $Re_l = ul/\nu$. Thus the difference between the largest and smallest length scales in turbulence increases as the Reynolds number increases. Since there are three spatial dimensions the number of grid points required to resolve turbulence increases as the cube of equation (4), *i.e.* as $Re_l^{9/4}$. When the time step (CFL) restriction is factored in one ends up roughly with computational cost increasing as the cube of the Reynolds number. This makes high Reynolds numbers impossible to simulate. However, many phenomena in turbulence appear to have a high Reynolds number asymptote (free shear layer growth rates, near wall mean profile etc.) and so numerical simulations at a 'high-enough' Reynolds number to capture these phenomena can already contribute greatly to understanding and model development.

We use the term 'direct numerical simulation' (DNS) to refer to computations where all relevant spatial and temporal scales are adequately resolved *for the given application.* Some applications, such as those requiring statistics involving higher derivatives, will require more resolution than others. The precise number of grid points needed depends also upon the numerical method. The preference for flows in simple geometries has been for spectral or high-order (greater or equal to 4th order) finite difference or finite volume methods. Detailed grid refinement studies show that away from walls grids of the order of 5η (recall that η is based on dimensional arguments alone) are sufficient for most purposes, such as prediction of mean flow and second moments of turbulence and all terms in the turbulence kinetic energy transport equation. A rule of thumb is that lower order methods, such as second order methods, require as much as a factor of two more points in all directions. However such methods may be quite efficient per grid point and more suitable for extension to complex geometry. Given that DNS on present-day parallel computers tend to be limited by run time rather than memory, there are some applications where such methods can be used. Upwind methods, unless they be of high order, are generally considered to be too dissipative for use in turbulence simulation (analysis in terms of the modified wavenumber is usually needed to check resolving powers of such methods). Unstructured grid calculations are expected to require more nodes in total to compute a given phenomenon, but as yet no estimates are available.

2.2 Validation procedures

All codes for simulation of turbulence need validation, and the lack of relevant exact solutions of the governing equations makes this more difficult. A list of suitable tests is as follows. Ideally all of these would be satisfied for a simulation to be accepted. In practice this is only true of one or two flows to date.

- Validate code against analytic solutions and asymptotic limits. This could include comparisons with exact solutions of the Navier-Stokes equations, boundary layer solutions, linear growth rates of small disturbances, etc.
- Carry out systematic grid resolution studies, varying resolution in one direction at a time and checking convergence for quantities of interest, e.g. turbulence statistics.
- Carry out systematic box size variations to check that the computational domain is large enough to contain the relevant flow physics. Decay of 2-point correlations to zero is a test that can be applied after a simulation has completed.
- Compute budgets of statistical quantities such as Reynolds stresses and check for balance.
- Compare results for the same problem between two different numerical methods, ideally from two separate, independently programmed codes.
- Carry out tests with a reduced time step to check for time discretisation errors.

For some flows the above criteria have been distilled down to a few 'rules of thumb'. For example in free shear layer calculations if one preserves say 6 decades of roll-off in the energy spectrum, one may reasonably expect good second moment turbulence statistics. For attached turbulent flow over walls grid spacings of $\Delta x^+ = 12$, $\Delta z^+ = 6$ and 10 points for $y^+ < 10$ are usually reckoned sufficient for good statistics related to budgets of Reynolds stresses.

2.3 The changing perspective of computer hardware

The usefulness of direct numerical simulations has increased with the rise in power of supercomputers, desktop workstations and personal computers. Simulations carried out in the early 1980s on Cray X-MP computers (for example isotropic turbulence at low Reynolds numbers, or the early stages of transition) can now be carried out on workstations. Larger computers can now be used to simulate higher Reynolds numbers and a wider range of geometries. During the Newton Institute programme several plots were shown of computer performance against time, showing improvements ranging from 10 times speed up every 5 years to 10 times speed up every 10 years. Recent measurements tend to be at the high end of this range and the curve shows no sign of asymptoting out in the near future. Bearing in mind the Reynolds number restriction on DNS given

in the last section this translates to a doubling of Reynolds number roughly every 5-10 years. The tendency in practice appears to be to use the increased performance to move to more complex flows, rather than just extend existing flows to higher Reynolds numbers.

Implementation of DNS numerical methods for massively parallel processing (MPP) entails additional considerations. The implementation of a spectral method described in [4] used a global transpose method, which involved the parcelling of small 'cubes' of data on each processor, labelling these with the address of the processor that requires the information, transferring the data, reading it by the receiving processor, and reconstructing the flow field. Both the PVM (Parallel Virtual Machine) and MPI (Message Passing Interface) libraries have been used successfully for this purpose. With the demonstrated success of such simulations on up to 256 processors on current machines, there appears little to prevent extremely large simulations in the near future on the ASCI architectures being developed in the US.

In passing, we note that another application of parallel processing to turbulence DNS is in the use of ensemble averaging to obtain averages for unsteady turbulence computations. In computing the temporal development of turbulence (and assuming that the time taken to converge to the base flow is not the critical element), one is often limited by the need to obtain ensemble averages by running the same code several times with independent initial conditions. This is easily done on a parallel computer by running multiple realisations at the same time. For example in one 256-processor job, 4 realisations each requiring 64 processors, or 8 realisations each requiring 32 processors, can be run at the same time.

2.4 Applications

Direct numerical simulations underpinned much of the theoretical work conducted at the Isaac Newton Institute, providing data that was used in a similar manner to experimental data for validation of theory. Here we can only give a flavour of some of this work and emphasise some of the new applications and post-processing ideas that were presented during the programme.

Durbin et al [5] presented results from DNS of bypass transition in which passing wakes triggered turbulent spots in a flat plate boundary layer. The simulations were modelled on an experimental/modelling study by Liu & Rodi (1991), which in turn modelled the environment in which transition on a gas turbine blade may occur. In the simulations travelling wakes, using data from a precursor simulation, were imposed upon a laminar boundary layer profile. Some disturbances were immediately ingested into the boundary layer as streaks, but did not cause transition. Instead turbulent spots developed further downstream, near the boundary layer neutral point, where disturbances from the free-stream entered the boundary layer. The terminology 'top-down' spots was used to describe these turbulent regions, which appear different to the classical 'bottom-up' spots, triggered by disturbances imposed at the wall. A qualitative explanation of why disturbances do not penetrate immediately through the

boundary layer was provided by Hunt using a rapid distortion idea of shear sheltering.

Vortex structure identification from DNS was a topic that recurred throughout the programme. There is at present no agreement (and may never be) on what constitutes a vortex. Perry (INI discussion) considers the only rigorous definition to be in terms of local critical point theory where foci and centres can be defined where complex eigenvalues of the local velocity gradient tensor exist. In DNS this can be plotted using a known discriminant. In practice this measure emphasises small scale structure and may not easily identify the largest-scale structures. Another measure for identifying vortices that is commonly used is low pressure. This certainly picks out the strongest structures, but may be ineffective in flows where mean pressure is changing spatially. Hussain (INI discussion) cited [7], in which a new definition based on the second eigenvalue of a combination of the strain rate and rotation rate tensors $S_{ik}S_{kj} + \Omega_{ik}\Omega_{kj}$. This was developed following a detailed critique of other measures and is based on an approximation (steady, inviscid) to an equation for the pressure Hessian $\partial^2 p/\partial x_i \partial x_j$. Kida presented an alternative definition using the pressure Hessian itself, together with a projection of the local flow on a plane perpendicular to the vortex axis, making use of a two-dimensional discriminant to ensure that low pressure cores correspond to swirling flow [8]. The resulting definition of 'vortex skeletons' is advantageous in that it does not require any user-defined threshold to be set.

Another set of turbulence structures that were studied during the programme were the streak structures of alternating low- and high-velocity fluid that are observed as the dominant structure in the sublayer of boundary layer and channel flows. The importance of such structures with relation to flow control was emphasised in talks by Hussain and by Lumley. There are, however, different ideas about the dynamical significance of streaks with respect to regeneration mechanisms of near-wall turbulence. Discussions during the programme have gone some way towards resolving these issues. In particular there was some agreement that the persistent low speed streaks usually visualised in experiments and simulation are stable streaks (an appealing argument being that if they were unstable one wouldn't see them). Additionally there was found to be agreement between three separate codes used to study streak instability. Results using the Schoppa & Hussain [9] streak profile were checked, and agreement was found between new data from Sandham and additional work of Uhlmann & Jiménez (following up on [10]) conducted during the programme. Streaks are formed by longitudinal vortex rolls. Once formed, the streaks may be amplified by more vortices passing by, or else diffuse away. If and when the streaks grow above a critical amplitude they will become locally unstable and a short-duration 'burst' will occur. Research remains active in this area, not least due to the important applications to modelling. A model that can predict the distinctive spanwise spacing of streaks $\lambda^+ = 100$ is still lacking.

Other examples of applications presented during the Symposium on Direct and Large Eddy Simulation included the following.

- Hüttl and Friedrich [11] presented results for turbulent flow in helically coiled pipes, where both the curvature and the torsion have a strong effect on flow structure.
- Sarkar [12] presented new results for the compressible mixing layer, confirming the reduction in pressure fluctuations observed by Vreman et al (1996) and adding a new distinction between early and late evolution of Reynolds stress anisotropy.
- De Bruin et al [13] showed results from simulations of spatially-evolving compressible turbulent mixing layers.
- Brethouwer & Nieuwstadt [14] used DNS to assess theories for spectra of passive scalar and its dissipation in isotropic turbulence. They report good collapse with Batchelor scaling at high wavenumber and also agreement with Kraichnan's model.
- Bouhadji & Braza [15] have carried out three-dimensional DNS of vortex shedding and near-wake evolution behind an aerofoil at $Re = 10000$.
- Thévenin & Baron [16] presented DNS of turbulent non-premixed flames using up to 9 species and 37 chemical reactions. They not surprisingly highlighted issues of post-processing the enormous amount of data relating to flame structure and chemistry that are produced by such simulations.
- Bury & Estivalezes [17] applied DNS to particle laden flows, computing mixing layer evolution with 64^3 particles at Stokes numbers ranging from 0.1 to 1000.
- Kawamura & Sumori [18] carried out DNS of a trapezoidal longitudinal ridge in a channel, finding good agreement with corresponding experiments and illustrating the feasibility of simulating flow in complex geometry.
- Kaltenbach [19] computed flow over a swept backward-facing step, including a parametric study of the effect of sweep angle and an examination of a sweep independence principle, which was found to hold for sweep angles up to 40°.

3 Large-eddy simulations

The large-eddy simulation method has its roots in predictions of atmospheric flows in the 1960s and like DNS has grown in importance as computers have increased in size and performance. At the time of writing commercial Computational Fluid Dynamics (CFD) codes are beginning to offer options to carry out LES and as a result the user community is expected to grow significantly in the next few years. As well as developing the technology, the challenge for academics is to try to communicate the requirements and limitations of the method to

users so that bad LES predictions do not replace bad Reynolds-averaged Navier-Stokes (RANS) calculations as the norm for predictions, to the dissatisfaction of all save perhaps the code vendors.

3.1 Background: Smagorinsky and dynamic models

Large-eddy simulation techniques are most usefully analysed by the use of explicit filtering, where we can define, for example in one spatial dimension, the filtered variable by

$$\overline{u}(x) = \int_{-\infty}^{+\infty} G(x - x')u(x')\mathrm{d}x'. \tag{5}$$

In practice, implicit methods are commonly used, but as we shall see later this blurs the distinction between numerical and modelling errors and prohibits useful analysis of schemes. Typical filters $G(z)$ include Gaussian and top-hat. The filtering operation can be applied to the Navier-Stokes equations (1) and (2) leading to

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{6}$$

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} \tag{7}$$

The stress term

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j \tag{8}$$

is not known a-priori and must be modelled.

The first, and still very widely used, model for τ_{ij} is the Smagorinsky model[1] which can be written in the form of an eddy viscosity

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\nu_T \overline{S}_{ij}, \tag{9}$$

where $\overline{S}_{ij} = 1/2(\partial \overline{u}_i/\partial x_j + \partial \overline{u}_j/\partial x_i)$ is the strain rate tensor based on the filtered velocity field. Note that the isotropic part τ_{kk} is a scalar unknown and can be combined with $\overline{p}$. The eddy viscosity is expressed as

$$\nu_T = (c_S \Delta)^2 \left|\overline{S}\right| \tag{10}$$

where

$$\left|\overline{S}\right| = \sqrt{2\overline{S}_{ij}\overline{S}_{ij}}. \tag{11}$$

Here Δ is the filter width and c_S the Smagorinsky constant, commonly set to a value cof around 0.1. If Δ is set equal to the grid spacing h then increasing the Smagorinsky constant may be thought of as a method of increasing filter width and reducing the contamination of modelling errors by numerical errors (Thomson, INI discussion).

[1]The form of which has its origins in the Richtmyer-von Neumann shock-capturing scheme (Leith, INI discussion).

Large eddy simulations of engineering flows are nowadays more likely to be based on dynamic formulations of the Smagorinsky model, originally developed by Germano et al (1991, 1992). These rest upon the Germano (1991) identity[2]

$$L_{ij} \equiv \widetilde{\overline{u}_i \overline{u}_j} - \widetilde{\overline{u}}_i \widetilde{\overline{u}}_j = \tau_{ij}^T - \widetilde{\tau}_{ij} \tag{12}$$

where $\widetilde{()}$ represents a second filtering operation, called a 'test' filter, performed with a larger filter width than $\overline{()}$ and $()^T$ denotes a quantity computed using the test-filtered LES velocity. The dynamic procedure can in principle be applied to any sub-grid model. For the Smagorinsky model given above we can equate L_{ij} to a term $c_S^2 M_{ij}$, where M_{ij} is given by

$$M_{ij} = -2\big(\tilde{\Delta}^2 \left|\widetilde{\overline{S}}\right| \widetilde{\overline{S}}_{ij} - \Delta^2 \widetilde{\left|\overline{S}\right| \overline{S}_{ij}}\big), \tag{13}$$

where $\tilde{\Delta}$ is the test filter width. Now the key step of dynamic modelling is to use Germano's identity to compute the value of c_S, leaving no free parameters in the problem, save the choice of filter widths. Operationally $\tilde{\Delta} = 2\Delta$ is usually used and combined with the procedure of Lilly (1992) which selects c_S to minimise the square of the error term $\epsilon = L_{ij} - c_S^2 M_{ij}$. This gives

$$c_S^2 = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}. \tag{14}$$

This procedure is not unique and also introduces the problem of how to carry out the averaging operation. For flows that are homogeneous in one or more directions it is usual to average in those directions. For more general flows local averaging and/or ad hoc limiters are required.

The model is especially well suited to transitional problems and relaminarisation, and can handle near-wall turbulence without additional corrections, so long as the near wall structures are reasonably well resolved (within a factor of four of a DNS, for example).

Jiménez & Moser [23] comment that the eddy viscosity models work surprisingly well given that the normalised correlation between stress and strain rate is only of the order of 0.2. They offer a partial explanation, pointing out that both Smagorinsky and dynamic Smagorinsky have an inbuilt self-adjustment property which makes them relatively insensitive to the precise choice of constant. If the constant is too low energy builds up in the high wavenumbers and the dissipation will be increased, and vice versa. The other key point from a practical point of view is that the models will always work well when the proportion of shear stress carried in the sub-grid model is significantly less than the shear stress of the large eddies.

This introduction to models has been of necessity brief. The reader is referred to recent reviews by Lesieur & Métais [24] and Härtel [25] for more details.

[2]This identity is known as the Leibniz identity in classical mechanics (Geurts, INI Discussion). A compact notation for LES is introduced in [49, 52] in which τ_{ij} is expressed as a commutator which shares many properties of the Poisson bracket.

3.2 Engineering and atmospheric applications

A summary of several LES test case workshops was given by Rodi during the INI Instructional Conference [26]. The case selected was flow around a square cylinder at $Re = 22000$ for which experimental data from Lyn et al [27] were available. The test case results demonstrated clear superiority of LES over RANS for a flow dominated by three-dimensional vortex shedding, even though the methods were significantly more expensive. No clear conclusions were reached regarding the relative performance of various subgrid models, but comparisons did identify bad numerical practices to be avoided in LES, such as excessive grid stretching and upwind schemes.

Other applications presented included LES of a jet into crossflow [28], and the development of unstructured grid LES for industrial applications by Laurence and co-workers [29]. At the Symposium on Direct and Large Eddy Simulation a limited number of applications of LES were presented.

- Mathey et al [30] presented results for flow over a wall-mounted array of cubes showing results for Smagorinsky, dynamic Smagorinsky and for no model at all. The small variation found suggests either that the flow is sufficiently resolved or that numerical errors dominate modelling errors.
- Kannepalli & Piomelli [31] carried out a spatial large-eddy simulation of a shear-driven boundary layer, the temporal counterpart of which has been studied by DNS previously. The sub-grid model was the localised dynamic eddy viscosity model.
- Garnier et al [32] carried out LES of shock wave interaction with homogeneous turbulence. Using DNS data as reference they find significant benefits of dynamic models compared to simple Smagorinsky.

Meteorological applications of LES were presented by Kerr [33], including discussion of the stochastic backscatter concept introduced by Leith [34]. This procedure is often employed in calculations of the atmosphere, partly to improve wall layer results [35] and partly to enable issues of predictability to be addressed (Leith, INI discussion).

3.3 New theoretical developments

Despite the successes of dynamic Smagorinsky modelling it possesses a number of shortcomings. The models usually employ local averaging or limiting so that c_S is positive everywhere and there is no backscatter from sub-grid to grid scale terms. A-priori tests, where actual sub-grid turbulence computed from DNS is compared with predictions from eddy viscosity modelling, show that the models are in this respect extremely poor. Filter widths as small as possible are employed, but this introduces another potential problem in that the filter and test filter may be placed in a part of the spectrum close to the grid scale where numerical errors may distort results. Bearing these facts in mind the hunt is still

on for better formulations for the sub-grid stress terms, making optimum use of information already contained in the simulation variables. Several strategies are reviewed in the next sections along with a rationale for mixed models and discussion of formal separation of numerical and modelling issues. The section ends with a wider discussion of the basic formulations of LES equations and links to other turbulence prediction methods.

3.3.1 Generalised tensor eddy diffusivity

One of the early models proposed for LES was the tensor eddy diffusivity model of Leonard [36, 37]. For a Gaussian filter

$$G(z) = \frac{\exp(-z^2/\sigma^2)}{\sigma\sqrt{\pi}} \tag{15}$$

Leonard has shown that the shear stress terms can be represented exactly by

$$\tau_{ij} = \sum_{k=1}^{\infty} \left(\frac{\sigma^2}{2}\right)^k \frac{1}{k!} \frac{\partial^k \overline{u}_i}{\partial x_l^k} \frac{\partial^k \overline{u}_j}{\partial x_l^k} \tag{16}$$

The full series would recover a 'DNS' result for τ_{ij} but is obviously not practical. Instead it was proposed to use only the first term as a subgrid model

$$\tau_{ij} = \frac{\sigma^2}{2} \frac{\partial \overline{u}_i}{\partial x_l} \frac{\partial \overline{u}_j}{\partial x_l} \tag{17}$$

By itself the model is insufficiently dissipative, and may become unstable. However, it can be combined with an eddy viscosity model to give good results (Vreman et al [38], Winckelmans et al [39]).

New developments with this model were presented by Carati et al [40], who have generalised the method for a much wider class of filters. They also discuss properties of the model with respect to reversibility of large scale structures. A detailed description and latest results from use of the mixed tensor diffusivity/dynamic Smagorinsky model are given in Leonard & Winckelmans [41].

3.3.2 De-convolution

Several different but related techniques are based on the suggestion that an approximate inversion of the filtering operation can be used to infer sub-grid stresses, without the use of a turbulence model at all. The inverse modelling approach is laid out in Geurts [42] and a related estimate method of Domaradzki & Saiki [43]. Here we focus on a new de-convolution methodology as described by Stolz & Adams [44] and Stolz et al [45].

Given a filtering operator G (so $\overline{u} = G * u$) an approximate inverse Q can be written as a truncated series

$$Q = \sum_{\nu=1}^{N} (I - G)^{\nu} \tag{18}$$

where I is the identity operator and N would typically be taken as 5. Stolz & Adams demonstrate the procedure using a family of non-negative filters based on Padé approximants. The cutoff of the filter can be adjusted according to numerical method so that the numerical errors at high wavenumbers do not contaminate the solution. The model is completed by the use of a secondary filter, only active above the cutoff wavenumber of the primary filter. This secondary filter removes energy from the system, but acts only at the highest wavenumbers. It does entail the introduction of a new constant, but the authors claim the results are not very sensitive to the precise choice of value. A priori tests and full calculations for channel flow are given in Stolz et al [45] which show good performance of the model for this standard test case.

A striking application of the approximate deconvolution procedure was given by Adams & Leonard [46] for shocks in the one-dimensional Burgers and Euler equations. Here model problems with discontinuities were solved without the use of explicit shock capturing algorithms by reconstructing the steep gradients by de-convolution. This opens up the possibility of a unified sub-grid treatment that can handle sub-grid turbulence or near-discontinuities in an efficient manner. There are obvious applications to the problem of shock wave interaction with turbulent boundary layers, for which current numerical methods are cumbersome and often inefficient.

Although still under development, these methods appear to be very efficient and show considerable promise for the future, when they may well pose a challenge to the established dynamic models.

3.3.3 Rationale for mixed models

Before discussing mixed models, we present the scale similarity model of Bardina et al [47]. In this method a second application of a filter is used to model the sub-grid stress term as

$$\tau_{ij} = \overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j \tag{19}$$

The model performs well in a-priori tests but in practical calculations is found to be insufficiently dissipative. This led Bardina et al to propose the first mixed model

$$\tau_{ij} = \overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j - 2(c_S \Delta)^2 \left|\overline{S}\right| \overline{S}_{ij}, \tag{20}$$

where scale similarity was combined with the usual Smagorinsky eddy viscosity to give a model that was sufficiently dissipative and could compute the backscatter effect.

Since the advent of dynamic modelling the idea of mixed models has again been tested. A comprehensive study of models for the transitional compressible mixing layer is given by Vreman et al [38]. In order of overall accuracy they had

1. dynamic mixed Smagorinsky plus scale similarity (both parts included in the dynamic procedure)

2. dynamic mixed Smagorinsky plus tensor eddy diffusivity (both parts included in the dynamic procedure)

3. dynamic Smagorinsky

4. scale similarity

5. tensor eddy diffusivity

6. Smagorinsky

The first three performed significantly better than the last three, while the last two were actually worse than no model at all (this would depend on numerical method). Further demonstration of the benefits of mixed models in other flows has been provided by Winckelmans et al [39] for decaying isotropic turbulence and channel flows, where a variant of model 2 above was used. Obviously there is much work to do in classifying the performance of all the different possible combinations of models across a wide variety of flows and important numerical issues have to be addressed, so that results can be applied in different codes (Vreman did use $\Delta = 2h$ in his calculations to reduce numerical effects, but this practice is rare). However a preliminary conclusion is that mixed models do well in both a priori and in a posteriori calculations.

A possible explanation for the good performance of mixed models was offered by Sarkar (see Shao, Sarkar & Pantano [48]) during the Symposium on Direct and Large Eddy Simulation. In this work a decomposition of the velocity field into a mean plus fluctuation $u = \langle u \rangle + u'$ is combined with the filtering operation. The shear stress is then written as $\tau_{ij} = \tau_{ij}^{\text{Rapid}} + \tau_{ij}^{\text{Slow}}$ where the 'rapid' part includes all terms with a mean velocity, and the 'slow' part includes terms only involving fluctuations

$$\tau_{ij}^{\text{Slow}} = \overline{u_i' u_j'} - \overline{u_i'}\ \overline{u_j'} \tag{21}$$

$$\tau_{ij}^{\text{Rapid}} = \overline{\langle u_i \rangle \langle u_j \rangle} - \overline{\langle u_i \rangle}\ \overline{\langle u_j \rangle} + \overline{u_i' \langle u_j \rangle} - \overline{u_i'}\ \overline{\langle u_j \rangle} + \overline{u_j' \langle u_i \rangle} - \overline{u_j'}\ \overline{\langle u_i \rangle}. \tag{22}$$

The slow part would always be present in LES, while the rapid part would only be active when mean velocity gradients were present, but would imply a rapid reaction of subgrid stresses to changes in the mean velocity profile. Two models were analysed by Shao et al. The scale similarity model was found to predict energy transfer effects corresponding to the rapid part, while Smagorinsky could represent the slow terms. This offers the first real rationale for mixed models and suggests that such models will be essential to compute flows involving rapid changes of mean flow or flows that are far from a production equal to dissipation equilibrium.

3.3.4 Numerical issues

Geurts [49] presents the current state of LES as a delicate balancing act between competing sources of error, both numerical and modelling. To separate the many sources of possible error he uses explicit filtering (following [50, 51]) and writes equations for general nonuniform filters, such as would be implicitly used in calculations on stretched grids. Additional terms appear due to the non commutation of the filter operator with the differentiation operator. In Geurts

& Leonard [52] it is postulated that not all the errors may be removed by using optimised filters such as in Vasilyev et al [53].

Demonstrations of typical magnitudes of errors are given in [49] for various ratios of filter width to grid spacing Δ/h. Using data from Vreman's simulations Geurts shows that for $\Delta/h = 1$ modelling errors are actually less significant than numerical errors for three different numerical schemes, while for $\Delta/h = 2$ numerical errors are reduced and modelling errors are large. In fact there is cancellation of errors taking place, since the sign of the modelling error may be opposite to that of the discretisation error. This illustrates that for LES one can expect that research groups using different numerics may report different, even opposite, conclusions about the comparative performance of models and filters. It will save endless applied test case workshops if the user community recognises this issue now.

3.3.5 New formulations and links to RANS

In a wide-ranging talk Germano [54] discussed the various different turbulence prediction strategies, including DNS, LES and RANS, and speculated about how these might be reformulated to provide a unified modelling strategy. RANS and LES fix a length scale in different ways. In RANS it is determined by $k^{3/2}/\epsilon$ or near a wall by κy, where κ is the Kármán constant, while in LES the smallest scale (comparable to a Kolmogorov scale) in a 'Smagorinsky fluid' (Muschinski [55]) is $c_S\Delta$. Hybrid strategies are often employed near walls by switching length scales from filter-width to wall distance as the wall is approached. Examples are the methods of Schumann [56], Mason & Callen [57] and the detached eddy simulation (DES) approach of Spalart et al [58]. Germano proposes a new formulation for grid-independent LES which is based on an imposed parameter that varies between 0 (DNS) and 1 (RANS) as the fraction of production carried by the LES is varied.

A variant of RANS modelling occurs when the equations are solved in a time-accurate manner, which may lead in some circumstances to unsteady solutions. For some examples (which may be pathological) the approach can lead to good predictions of turbulence flow. An example is Rayleigh-Bénard convection, an example shown by Hanjalić (based on [59]). A tendency in the RANS community has been to introduce new names for this method. However terminologies like very large eddy simulations (VLES) are considered inappropriate, given that connections to LES are weak. It was generally agreed among participants that 'unsteady RANS' was the best term to use for these kinds of simulations.

A development from recent analysis is the Navier-Stokes alpha (NS-α) model, an excellent introduction to which is given by Holm [60]. A modified Kelvin's theorem is assumed to hold, using integration around a loop moving with a spatially filtered velocity. Equations comparable to the Navier-Stokes equations are obtained as

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{23}$$

$$\frac{\partial u_i}{\partial t} + \overline{u}_j \frac{\partial u_i}{\partial x_j} + u_j \frac{\partial \overline{u}_j}{\partial x_i} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j}, \tag{24}$$

where $\overline{u}_i$ is a filtered form of u_i, or inversely

$$u_i = \overline{u}_i - \alpha^2 \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j}. \tag{25}$$

The steady solution of the NS-α equations is identified with the mean turbulent flow. Chen et al [61] show that for channel and pipe flows the results are in good agreement with experiments over a wide range of Reynolds numbers. Numerical simulations of isotropic decaying turbulence with the NS-α equations are given by Chen et al [62], demonstrating some features of the model. The length scale α is fixed according to the smallest scale required to be accurate from the simulation. Compared to Navier-Stokes the NS-α model shows a roll-off in energy spectrum of k^{-3} rather than $k^{-5/3}$ at high k. Thus fewer modes are required to compute the same number of decades of the energy spectrum, with considerable savings in computer time compared to DNS of the Navier-Stokes equations. A nice feature of the system is that from the beginning it separates the physical model (given above) from the numerical techniques of solution. Additionally it appears that more rigorous analysis can be done with the model than with the full Navier-Stokes equations, which should prove to be of benefit. The model is not the same as conventional LES since an equation like (24) for $\overline{u}_i$ would include time-dependent terms on the right hand side, which has not been tried in LES.

4 Conclusions

4.1 Guidelines for application of current LES technology

The paper by Geurts & Leonard [52], which emerged from interactions at the Newton Institute, concludes with guidelines for careful application of existing LES technology and addresses the issue of whether LES is actually ready for complex engineering calculations yet. The lack of a definitive 'yes' in their conclusions should be taken as a warning to those who propose that LES will replace RANS for practical calculations at high Reynolds numbers over the foreseeable future. Of course many applications at lower Reynolds numbers will be amenable to LES (wall-resolving) and even DNS.

The Geurts-Leonard guidelines are worth summarising again here to show how a new user may begin to gain trust in results obtained from a present-day LES code (The validation procedures given for DNS in section 2.2 are also relevant).

- Validate the code against simpler theory and DNS databases.
- Use smoothly varying near-orthogonal grids and avoid dissipative numerical methods.

- Vary numerical and physical parameters (grid, box size, numerical method etc.)
- Use dynamic modelling (mixed models are especially recommended).
- Use explicit filtering and incorporate LES predictions at different Δ/h into the flow analysis.

The field is moving rapidly and new techniques such as deconvolution and inverse modelling may offer improved performance. It is recommended that users keep in touch with the literature as it develops and not rely solely on products from software vendors in this highly complex field.

4.2 Key issues and requirements for future research

All the topics presented in section 3.3 need to be further developed to arrive at a consensus of good modelling and numerical practice.

One area that has not been discussed so far is near-wall treatments, where progress is slow. A common practice at present in the engineering community is to use dynamic models and resolve near-wall structures such as streaks. A factor of four less resolution in all directions can be used relative to DNS. This represents a considerable saving. However the scaling with Reynolds number is such that it is impossible to extend the method to applications such as flow over an aircraft wing. Such simulations are something of a 'poor man's DNS'. They are not sufficiently resolved to provide reliable data for investigations of flow physics and model validation (although they are undoubtedly a better representation of the flow physics than RANS models), while at the same time they are not demonstrating LES technology for applications, since the Reynolds numbers are still low. Better wall treatments are definitely needed to enable applications of LES to higher Reynolds numbers. Test cases involving DNS of flows with turbulent separation and reattachment should be of some assistance in developing models that have some useful range of applicability. Another hope is that some of the fundamental knowledge being gained about near-wall turbulence mechanisms and control strategies can be applied to LES modelling.

There is justifiable interest at present in building new experimental facilities that can extend to very high Reynolds numbers. The Princeton 'superpipe' has provided mean velocity data that has greatly stimulated theoretical work (although it is disappointing that measurements do not appear to extend below $y^+ = 1000$ at the highest Reynolds numbers). In connection with DNS we should note that the highest Reynolds number boundary layer DNS is still that of Spalart [63] at $R_\theta = 1410$. For its day this was an extremely large calculation, but hardware has already progressed to the point where one can conceive of further calculations at $R_\theta = 2820$ and 5640. Such simulation would complement experiments by providing complete datasets for Reynolds number trends to be studied and compared with theoretical predictions. A concerted effort perhaps involving international collaboration could be appropriate for such an exercise.

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