The emerging role of large eddy simulation in industrial practice: challenges and opportunities

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That class of methods for treating turbulence gathered under the banner of large eddy simulation is poised to enter mainstream engineering practice. There is a growing body of evidence that such methods offer a significant stretch in industrial capability over solely Reynolds-averaged Navier–Stokes (RANS)-based modelling. A key enabling development will be the adaptation of innovative processor architectures, resulting from the huge investment in the gaming industry, to engineering analysis. This promises to reduce the computational burden to practicable levels. However, there are many lessons to be learned from the history of the past three decades. These lessons should be analysed in order to inform, if not modulate, the unfolding of this next cycle in the development of industrial modelling capability. This provides the theme for this paper, which is written very much from the standpoint of the informed practitioner rather than the innovator; someone with a strong motivation to improve significantly the competence with which industrial turbulent flows are treated. It is asserted that the reliable deployment of the methodology in the industrial context will prove to be a knowledge-based discipline, as was the case with RANS-based modelling, if not more so. The community at large should collectively make great efforts to put in place that knowledge base from which best practice advice can be derived at the very start of this cycle of advancement and continue to enrich it as the cycle progresses.

Keywords: Reynolds-averaged Navier–Stokes turbulence modelling; large eddy simulation; hybrid RANS–LES; best practice; knowledge base; industrial capability

1. Introduction

Fluid flow pervades much of human experience and endeavour, from the bloodstream flowing within our bodies to the weather systems that surround us, and a great deal in between such as all the industrial processes, transport vehicles and power systems that are vital pillars of modern society and economic well-being. We aspire to model and simulate these systems with ever-increasing precision so as to be able to better understand or control them, or to improve their functionality and performance. The richness and complexity of these fluid systems and the questions they pose are, in large part, because of the fact that

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the majority of them are turbulent. (Even in blood flow, turbulence is a key concern. Vascular implants can cause turbulence increasing the risk of thrombosis.) So there is an overarching requirement for treatments of turbulence that are both competent and practically feasible across a wide range of applications. A great deal of human capital has been invested in this quest over the past 30 years. Many take the view that the fruits of this investment have been disappointing, particularly in the field of engineering design and assessment. Now that class of treatments known as large eddy simulation (LES) is poised to enter mainstream engineering practice. There are many lessons to be learned from the history of the past three decades. These lessons should be analysed in order to inform, if not modulate, the unfolding of this next cycle in the development of industrial modelling capability. This provides the theme for this paper. It is written very much from the standpoint of the informed practitioner, rather than the innovator; someone with a strong motivation to improve significantly the competence with which industrial turbulent flows are treated. The views and opinions expressed are personal, but very much founded upon the author’s interaction with the community at large.

2. Current industrial practice

It is generally accepted that turbulent fluid behaviour is governed by the Navier–Stokes equations. However, as is well known, attacking turbulence directly through these equations is not practically feasible. The range of length and time scales that must be captured is such that computational costs scale as $Re^3$ ($Re$ denotes the Reynolds number of the equipment or system) and most engineering equipment operates at $Re \sim 10^6–10^7$. Indeed, it has been estimated that direct numerical simulation of the flow over an aircraft using a computer with teraflop performance would take several thousands of years (Moin & Kim 1997). Hence turbulence must be modelled in such a way as to bring the costs down to a practicable level. From the very early days of industrial computational fluid dynamics (CFD) practice to the present time, the treatment of turbulence has been based on closure models of the Reynolds-averaged Navier–Stokes (RANS) equations. The limitations of the available computer power have rendered this the only feasible option, although the complexity and sophistication of the closure models deployed have increased in line with advancing power. An enormous amount of human capital and ingenuity has been invested in this enterprise over the past few decades. However, to date, no practicable model or class of models has emerged that is competent across a broad range of flows featuring diverse states of strain. There is, it would seem, no universal statistical state of turbulence. Over 100 RANS models or model variants have now been published. Many of these variants have been devised to fix a problem in a preceding model, but few are widely successful beyond that class of flows against which they are calibrated.

This vast cornucopia of capability is such that there is probably a model that can do a reasonable job for one’s particular application providing best practice is followed, and the results are interpreted from a position of deep knowledge. This best practice and knowledge is not widely available in the community of industrial practitioners. Indeed, very few people, if any, hold the knowledge.
of how to best match which model to which flow application and how to interpret the results and limit uncertainties affecting engineering design. As such, inappropriate choices are frequently made. A significant proportion of industrial applications deploy the standard $k$–$\varepsilon$ model with wall functions (SMWF). For example, Formula-1 car designers run aerodynamic simulations on meshes of many millions of cells (often hundreds of millions), which resolve the geometry in exquisite detail, and yet they generally opt for this model. It is known that SMWF cannot capture separation and subsequent wake behaviour among many other recognized inadequacies (Casey & Wintergerste 2000).

The last decade of the last century witnessed a minor renaissance in the advancement towards industrially competent turbulence models with the appearance of the model of Spalart & Allmaras (1992), Menter SST (Menter 1994), Durbin’s V2F model (Durbin 1991) and a number of EARSM/nonlinear eddy viscosity models. These improved markedly the ability to model complex industrial flows, particularly wall-attached flows up to and just beyond separation. However, all models devised to date appear unable to predict adequately post (gross) separation behaviour, including reattachment and recovery. They also struggle to capture complex jet behaviour (Tucker 2008). Can further investment in RANS model development push through these barriers, or is it necessary to simulate the dynamics of the larger energy bearing eddies in order to deliver a substantial stretch in capability? If so, can this be achieved by resorting to unsteady RANS (URANS) treatments or very large eddy simulations? The RANS equations are generated by time-meaning the terms in the Navier–Stokes equations over a period that is at least as long as the turnover time of the largest eddies. It must surely follow that the resulting Reynolds stresses cannot resolve information concerning the dynamics of smaller, higher frequency eddy structures. Hence, in the opinion of the author, these stresses should be modelled using length and time scales of the order of only the very largest eddies. As a consequence, URANS cannot then simulate the dynamics of a sub-range of eddy scales. Of course, one can choose to adopt closures constructed on much smaller scales (e.g. as in detached eddy simulation (DES; Spalart 2009), or Menter’s SAS model (Menter & Egorov 2004, 2005)), but surely the result can no longer be classed as RANS modelling.

3. Knowledge capture and best practice

As already pointed out, more than 100 RANS turbulence models or model variants have emerged over the past few decades, and fresh ones continue to appear, which try out new ideas or which fix inadequacies discovered in predecessors. These are then validated over a relatively narrow range of flows. Confusion tends to reign in industry. Which of these models is the best for a given application in terms of competency, robustness and affordability? How far can they be pushed outside their range of validation? How should other modelling choices be made (e.g. mesh resolution, boundary condition set-up, etc.) so as to ensure that competence, which may well have been demonstrated under entirely separate conditions, is not undermined by the impact of other sources of error on model performance? It is now generally accepted that there is no universal statistical state of turbulence and, as such, no (single-point) closure is
likely to emerge that is competent across a wide class of industrial flows spanning a broad spectrum of states of strain (Hunt & Savill 2005). The author is of the view that future investment in RANS modelling should be strategically diverted to the challenging task of assembling and structuring knowledge and guidance in a form that can provide answers to the above questions. A start has been made towards this objective. An enormous body of knowledge has been generated across all industrial sectors, largely as an outcome of numerous validation and comparison exercises. However, this body is somewhat dispersed, is relatively underused and tends not to migrate across sectors. The QNET-CFD project set out to pull together this important resource, to critically examine and filter it, and then to structure it into a form from which well-founded best practice advice could be derived (Hutton 2005). The result is the QNET-CFD Knowledge Base (http://eddie.mech.surrey.ac.uk). This is application centred, facilitating the identification of appropriate knowledge and advice for specific industrial purposes. It has a hierarchical structure organized around: Application Areas such as built environment, external aerodynamics, turbomachinery, combustion, heat transfer, etc.; Application Challenges that are realistic industrial test cases, which can be used to judge the competency and limitations of CFD for a given application area; and Underlying Flow Regimes that are generic, well-studied test cases capturing important elements of the key flow physics encountered in one or more application challenges. At each level, comprehensive, evidence-based best practice advice and guidance is set out. By this means, advice derived from very well-studied underlying flow regimes is lifted into the more complex level of the parent application challenge. This prototype Knowledge Base must now grow and be continuously enriched as domain knowledge and capability evolve.

4. The emerging role of LES

(a) Challenges

Designers of engineering products and equipment rely increasingly on computational simulation to optimize performance against constraints of escalating complexity. To meet the challenge, they aspire to explore and characterize ever-expanding regions of design space. As a consequence, CFD is being used to study flow regimes that are beyond the competency of RANS modelling (massively separated flow, afterbodies, wind flow within the built environment, noise generation from vehicle airflow, fine-scale mixing, transition, etc.). Can LES emerge as a practical industrial design tool to bridge this gap, and if so when? LES has, in fact, already achieved a certain level of industrial maturity in applications for which the influence of the wall on the essential flow physics is not significant, such as when the wall acts simply as a containment in say process equipment, or the flow is uncontained (i.e. plumes, flames, jets, etc.). However, a great deal of engineering design is devoted to optimizing geometries such as airframes, gas-turbine blade passages, marine platforms, heat transfer surfaces, etc. Then the influence of the wall on flow behaviour is likely to be crucial. In particular, the small streak structures at the wall must be resolved in order to capture the generation and sustenance of turbulence in the boundary layer. These structures are very fine indeed with length, width and height of order 1000, 20 and 30 wall units, respectively. The number of near-wall grid
points required scales as $Re_T^2$ and the cost becomes prohibitive at realistic Reynolds numbers. At the end of the last century, it was estimated that $10^{11}$ grid points and $5 \times 10^6$ time steps are necessary to simulate the flow over an aircraft wing, and this would not be a practical proposition for several decades to come (Spalart et al. 1997).

It has been proposed that this problem can be dealt with by adopting a hybrid approach. As already mentioned, a number of fairly simple RANS turbulence models have emerged, which perform well in wall-attached boundary layers up to and just beyond the point of separation. Thus a promising and practicable compromise is to treat the wall near region with (unsteady) RANS and the wall remote and separated regions with LES. This hybrid RANS–LES approach has been the subject of much research in recent years and has scored some very notable successes in flows of industrial complexity. The most popular variant at present is the DES method first proposed by Spalart et al. (1997) and further explored and developed by others (Strelets 2001; Spalart 2009). The basic idea is to select an appropriate RANS model for the near-wall behaviour (e.g. Spalart and Allmaras or Menter SST) and arrange for the length scale in the dissipation terms to adopt a value proportional to the local mesh spacing as distance from the wall increases. If this is done judiciously, it can be shown that, for equilibrium turbulence, the wall remote model is equivalent to that of Smagorinsky except perhaps for the choice of model constant.

So how practicable are hybrid methods for industrial application in the short to medium term? Can they mature to become an industrial workhorse displacing RANS methods for a broad class of industrial flows? Clearly, the computational cost is considerably higher than that incurred with (steady) RANS. Outside the wall region, the mesh must consist of regular, isotropic cells, with smooth, fairly gradual spatial change in resolution in order to minimize the erosive effect on numerical dissipation. In the important flow regions (i.e. where turbulent processes are key drivers of overall flow phenomena), the dynamics of the complete large-scale range must be captured. The time step must be of the order of the turnover time of the smallest resolved eddies and the simulation must be run for a period sufficiently long to establish fully developed statistics. The author, after consultation with colleagues who are experienced practitioners of DES, estimates that a hybrid solution to a problem is of the order of $10^3$–$10^4$ times more expensive than a steady RANS solution. It is difficult to be more precise because the computational effort depends strongly upon the complexity of the problem, the quality of the solution sought and indeed the expertise of the person running the solution.

Even if computational performance ceases to be a prime barrier in the medium term, a large number of complex issues, rich in variety, remain to be addressed to establish industrial maturity. A limited, far from complete selection is listed below. These have been selected from the viewpoint of the industrial practitioner.

— How should the RANS–LES interface be set up and how can this be positioned automatically? The optimal location will of course depend upon the flow physics of the problem in hand.
— How can the information exchange across the interface best be treated (seeding of the LES from the RANS region and filtering of the LES to provide an appropriate condition on the RANS region)? This issue is handled implicitly and opaquely in the DES variant.

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— Which numerical scheme is appropriate for each region and how should they be blended?
— Unlike RANS, the mesh is now part of the model and must be designed to minimize erosion of physics by numerical error. What new procedures and practices are required?
— What are the key off-surface flow regimes that strongly influence engineering performance, and how can the sufficiency of mesh resolution be ensured in such regimes?
— Given a mesh resolution within a given flow regime, could/should model constants be set to compensate for the level of numerical error? Indeed, by adopting implicit LES methods, can physical modelling be entirely dispensed with and under what conditions?
— How should the time step be selected and how long should the simulation run for a given application?
— How are initial and inlet conditions generated, which correctly seed the simulation?
— How should the engineer deal with the huge amount of data generated by the simulations? What information should be extracted and how can this best be done?
— As the field of research becomes ever more topical, many new variants, flavours and practices are and will continue to emerge (Sagaut et al. 2006). How can the comparative benefits and limitations of these be established across the full range of applications?

(b) Opportunities

There is a growing body of evidence that hybrid methods do offer a significant stretch in industrial capability over RANS alone. Given its current popularity, much of this evidence has been generated using DES (Peng & Haase 2008; Spalart 2009). Post-massive separation behaviour can be adequately captured, including recovery following reattachment. The massively separated flow over a complete F-15 jet has been simulated by Forsythe et al. (2004) yielding moments and forces that are accurate to within 6 per cent. A wide spectrum of promising applications spanning wing high-lift systems, helicopters, combustors and afterbodies are reported by Peng & Haase (2008). Hybrid methods such as DES are proving particularly enabling in aero-acoustic applications such as cavity aero-acoustic resonance (Mendonca et al. 2003; Ashworth 2008) and noise generation from airflow over vehicles (Mendonca et al. 2002).

What are the opportunities for bringing LES and hybrid methods in particular into frontline industrial practice in the near to short term and how should the process be managed? It was suggested earlier that an increase in commonly available computer power well in excess of $10^3$ is required for this to be possible. Over the last two decades of the previous century, a combination of processor and algorithm development yielded an approximately $10^6$ improvement in CFD computational performance (J. Appa 2008, personal communication). This needs to be repeated but in a shorter time. Coincidentally, hardware and architecture advancement is at a cusp point. Nearly all research and development is being invested in generic off-the-shelf technology, and this technology is being driven largely by the gaming industry. Special bespoke systems for computational engineering are probably a thing of the past. Most of the top 500 systems in the...
world now use off-the-shelf processors. The density of on-chip transistors is reaching a limit set by the difficulty in managing heat generation. For this reason, the clock frequency of conventional processors is remaining constant or even decreasing. On the other hand, computer graphics hardware is advancing rapidly and is capable of delivering 100 times the performance of high-end conventional processors. Currently, the world’s most powerful computer, the Los Alamos RoadRunner, can perform $10^{15}$ operations s$^{-1}$ (one petaflop), using a processor designed for the Sony PlayStation. However, in order to exploit this power, algorithms must be highly parallel. This is the opportunity. If, in the short to medium term, highly scalable parallel algorithms can be developed for solving the Navier–Stokes equations, then the requisite increase in computational power can be brought on stream.

Finally, as LES and hybrid methods are brought to industrial maturity, what lessons, if any, should be drawn from the experience of the past decades of treating turbulence? It can be predicted, with a fair degree of certainty, that practitioners will be called upon to exercise great skill and knowledge in order to design and set up the problem analysis; to navigate successfully the plethora of decisions and choices that will be needed to complete the model definition and run the simulation; and to interpret the results from a position of confidence and trust. The reliable deployment of the methodology in the industrial context will prove to be a knowledge-based discipline, as was the case was with RANS-based modelling, if not more so. The community should avoid a repeat of history, and should collectively make great efforts to put in place that knowledge base from which best practice advice can be derived at the very start of this cycle of capability improvement. In the absence of such guidance founded on sound knowledge, the methods will be deployed by many, perhaps the majority, of practitioners inappropriately, inviting an outcome where value derived from the investment made is held in question.

5. Concluding remarks

Over the past few decades, as innovator and practitioner alike laboured with great ingenuity to refine and deploy RANS-based solutions to complex practical problems, LES-based methods beckoned as an enabling and attractive alternative, but always remained stubbornly just over the horizon. Now, these are fully poised to enter mainstream practice. A key enabling development is the adaptation of innovative processor architectures, resulting from the huge investment in the gaming industry, to engineering analysis. However, in order to take advantage of this paradigm shift, highly scalable, parallel algorithms for solving the Navier–Stokes equations must be crafted. This should be regarded as a high priority.

There is a growing body of evidence that the LES and hybrid class of methods will deliver a substantial stretch in industrial competency and capability. However, it is equally becoming apparent that the reliable and trustworthy deployment of this class in the industrial context will be very much a knowledge-based discipline, just as much as RANS-based modelling proved to be, if not more so. The lessons of history must be heeded. The community as a whole, researchers, end-users and providers of funds, should invest in the construction and dissemination of the appropriate knowledge base at the very start of this cycle of advancement and continue to enrich it as the cycle progresses.
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