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High-performance computing in computational fluid dynamics: progress and challenges

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Computational fluid dynamics (CFD) is by far the largest user of high-performance computing (HPC) in engineering. The main scientific challenge is the need to gain a greater understanding of turbulence and its consequences for the transfer of momentum, heat and mass in engineering applications, including aerodynamics, industrial flows and combustion systems. Availability of HPC has led to significant advances in direct numerical simulation (DNS) of turbulence and turbulent combustion, and has encouraged the development of large-eddy simulation (LES) for engineering flows. The statistical data generated by DNS have provided valuable insight into the physics of many turbulent flows and have led to rapid improvements in turbulence and combustion modelling for industry. Nevertheless, major challenges remain and the computational requirements for turbulence research, driven by well-established physical scaling laws, are likely to remain at the limit of the available HPC provision for some time to come.

Keywords: direct numerical simulation; large-eddy simulation; Reynolds-averaged Navier–Stokes simulation; turbulence; turbulent combustion

1. Introduction

Computational fluid dynamics (CFD) is now well established, both as a powerful tool for fundamental research and as an invaluable aid to industrial design. The foundations for modern CFD were laid about 30 years ago (Harlow & Welch 1965; Orszag 1969; Launder & Spalding 1974) and the subject has progressed mainly in line with the increasing availability of computing power. A major source of difficulty in the simulation of fluid-flow phenomena arises due to the very large range of length- and time-scales that occurs even in nominally simple problems. Examples of small-scale flow structures that occur within a much larger flow field include the viscous boundary layer close to a flat plate in laminar flow, the shock-wave patterns emanating from the leading edge of a wedge in supersonic flow, and the bright yellow soot-formation zone in a standard laboratory bunsen flame. All of these phenomena share the property that their thickness is very much smaller than their extent in the other two spatial dimensions. If the flow is turbulent, then the range of length- and time-scales is not only large but also comprehensively filled with eddies at all scales and in all three dimensions. Inevitably, many of these small-scale phenomena do not occur

One contribution of 15 to a Discussion Meeting 'New science from high-performance computing'.

in isolation but instead are present and must be simulated in combination. Also, in most problems of industrial interest the geometry of the flow domain is necessarily complex and contains a broad range of length-scales, such that representation of the geometry itself is a significant computational task.

The Navier–Stokes equations governing fluid flow have been known for over 100 years. Analytical solutions have been found for only a handful of very simple problems, and therefore numerical analysis is unavoidable in general. Standard CFD practice involves the discretization of the Navier–Stokes equations on a grid constructed from a set of points in the domain of interest. Finite-volume methods are favoured for most engineering simulations due to their excellent conservation properties, while high-accuracy finite-difference methods are used mainly for well-resolved calculations. In either case, the discretization procedure is designed for consistency, such that the errors incurred will vanish rapidly as the spacing of the grid points is reduced towards zero. Nevertheless, the total number of grid points that can be handled depends on the capacity of the available computing hardware and is necessarily limited. Clearly, this constraint applies also to the need for resolution of small-scale phenomena. For example, the number of grid points required to resolve a boundary layer on the wing of an airliner may not be affordable in the context of a complete-aircraft simulation and alternative strategies are required.

In practice, the accuracy of discretization schemes has proved less restrictive than the resolution requirements of small-scale phenomena. Where the location of a small-scale phenomenon is known in advance, it is possible to make use of a static but non-uniform distribution of grid points. This is now standard practice in resolving boundary layers, which are naturally associated with solid walls. Where the exact location is not known, or the phenomenon is transient by nature, it may be possible to make use of known physics to capture the phenomenon despite inadequate resolution. This approach is generally used for shock waves, where the thickness may be no more than a few molecular mean free paths but the jump conditions across the wave are well understood. In the case of turbulence—where the phenomenon is essentially space-filling, transient and not well understood—there is no alternative for practical problems but to make use of statistical modelling techniques.

Turbulence modelling is a notoriously difficult subject lacking in a strong philosophical underpinning and beset with questionable physical assumptions. Nonetheless it is essential, since the overwhelming majority of practical fluid-flow problems involve turbulence and hence are affected by the turbulent exchange of momentum, heat and mass. Full resolution of the turbulent flow field in most industrial devices remains impractical, and the standard approach is to make use of Reynolds averaging. For statistically stationary flow fields a time average over a period much longer than the correlation time of the turbulence is sufficient (Reynolds 1895) and yields a modified set of governing equations known as the Reynolds-averaged Navier–Stokes (RANS) equations. For non-stationary flows a concept of phase averaging (for statistically periodic flows) or ensemble averaging over a large number of realizations is employed instead (Pope 2000). The averaging process removes all small-scale phenomena below the mean-flow length-scale, but the RANS equation set is unclosed due to the nonlinearity of the convection terms. A closure model is then required to represent the information that has been lost. Development of closure models for the RANS approach has occupied many researchers for about 30 years, and the standard was set quite early by the so-called k–ε model (Jones

& Launder 1972) and the rather more sophisticated Reynolds stress model (Launder *et al*. 1975). The strengths and weaknesses of these models by now are well known, and a great deal of research has been devoted to their improvement and extension.

An alternative approach which is now gaining in popularity due to increased computer power is large-eddy simulation (LES). As the name implies, LES attempts to resolve explicitly the large-scale flow features, leaving the small-scale features unresolved. A formal spatial filtering operation is applied to the Navier–Stokes equations, using a filter width that can be resolved on an affordable computational grid (Rogallo & Moin 1984). Once again, unclosed terms arise due to the nonlinearity of the Navier–Stokes equations, and a closure model is required to represent lost information at the sub-grid scale. Early development of LES and the accompanying sub-grid closure modelling was aimed mainly at weather prediction (Smagorinsky 1963). In this context, and in engineering flows, the principal advantage of the LES approach over the RANS approach is that most of the turbulent energy-containing motions in principle can be explicitly resolved. The principal disadvantage of LES is that the computational cost is much greater than for RANS, since the simulation is necessarily three dimensional and time dependent owing to the nature of turbulence, and it is no longer possible to take advantage of statistical symmetries or stationarity. Thus, for industrial purposes, RANS remains a popular choice.

The impact of high-performance computing (HPC) on the field of CFD has been felt in several ways. It has become possible to carry out RANS simulations of much more complex problems involving unsteadiness, coupled physics and complex geometry. LES has become feasible for simple industrial problems and is under active development for application to more realistic geometries. Nevertheless, both approaches are being held back by the need for better models of small-scale turbulence and related effects, and by the computational cost of very large simulations. Industrial users require rapid turnaround and high throughput in order to integrate advanced CFD into the design cycle. Thus the greatest and most immediate impact of HPC on CFD has been the advent of direct numerical simulation (DNS), in which all flow features are explicitly resolved and no modelling is required. DNS depends entirely on the availability of very large computing power, and is restricted to small problems involving very simple geometry. Nevertheless, its influence has been enormous, thanks to the level of accuracy that is attainable and the wealth of detail that is available. DNS has resulted in the development of a new generation of discretization schemes and solution algorithms with emphasis on high accuracy and high resolution. Data derived from DNS has been used extensively to calibrate existing turbulence models and to develop novel approaches, and numerical flow visualization based on DNS has allowed several turbulent interaction mechanisms to be elucidated (Kim *et al*. 1987). DNS has been of particular value in combustion, where turbulence–flame interaction modelling has been greatly strengthened as a direct result of the availability of DNS data (Bray & Cant 1991; Echekki & Chen 1996; Vervisch & Poinsot 1998; Cant 1999).

The purpose of the present paper is to summarize the impact of HPC in CFD, by giving some examples drawn from the UK engineering community. UK interests in computational engineering are served by the High Performance Computing in Engineering Steering Group (HPCESG) also known as CCP12. Three subject-based consortia associated with HPCESG are the UK Turbulence Consortium, the LES-UK Consortium and the Consortium on Combustion for Engineering Applications. All involve major usage of HPC and their work serves to illustrate recent progress in CFD together with some of the major challenges.

2. Direct numerical simulation

The purpose of DNS is to simulate a flow in all its detail, without the need for closure modelling. DNS techniques have been applied mainly to turbulent flows and have proved especially useful in turbulent combustion. There is an overriding need for adequate resolution of the smallest features in the flow. In turbulence the smallest scales are the Kolmogorov length- and time-scales of the smallest eddies; in combustion the smallest scales may well occur within the local structure of the flame. The key parameter describing the range of length- and time-scales is the Reynolds number of the flow, and it is important in DNS that this be made as large as possible in order to give confidence in the generality of the results. Accepted scaling laws for turbulence (Pope 2000) then define the required computational grid size. For reasonable Reynolds numbers the computational grid in DNS contains a very large number of points. Since in addition DNS is necessarily three dimensional and time dependent it is clear that the computational cost of DNS is enormous. The need for resolution also defines the type of discretization schemes required for DNS, since standard low-order schemes generally offer inadequate resolution of small-scale (high-wavenumber) features. Early DNS was based largely on Fourier spectral methods (Orszag 1969), which offer excellent resolution but suffer from a lack of flexibility in the specification of boundary conditions. Modern practice is based on high-order finite differences, using either compact Padé schemes or high-order explicit centred schemes (Lele 1992). DNS of flows involving shock waves are especially demanding, and discretization methods based on entropy-splitting have been developed for this purpose (Yee *et al*. 1999). In DNS of turbulent combustion some compromises are necessary, since a fully resolved computation of turbulent flow coupled to a full chemical reaction mechanism for the oxidation of a realistic hydrocarbon fuel is not yet feasible. Where chemical or molecular diffusive effects are of interest it is possible to carry out two-dimensional simulations with full treatment of the chemistry (Echekki & Chen 1996), and where flame–turbulence interaction is of interest, simulations in three dimensions are essential and a simplified chemical treatment must be used (Jenkins & Cant 2001). Accurate and efficient time-stepping algorithms are particularly important in DNS, and low-storage Runge–Kutta schemes are favoured (Wray 1990). In combustion DNS the stiffness of the chemical reaction scheme is often a major source of difficulty, and adaptive Runge–Kutta schemes are under development (Kennedy & Carpenter 2001).

Examples of current DNS practice are shown in figures 1 and 2. In figure 1, results are shown for DNS of transonic flow over a bump in the lower wall of a channel (Ashworth *et al*. 2002). The flow is from left to right, and contours of velocity magnitude, Mach number, pressure, density and internal energy are shown. A shock wave is clearly visible as a near-vertical dark line a short distance downstream of the trailing edge of the bump. A turbulent boundary layer is also evident, beginning close to the bump trailing edge and developing downstream. The Reynolds number

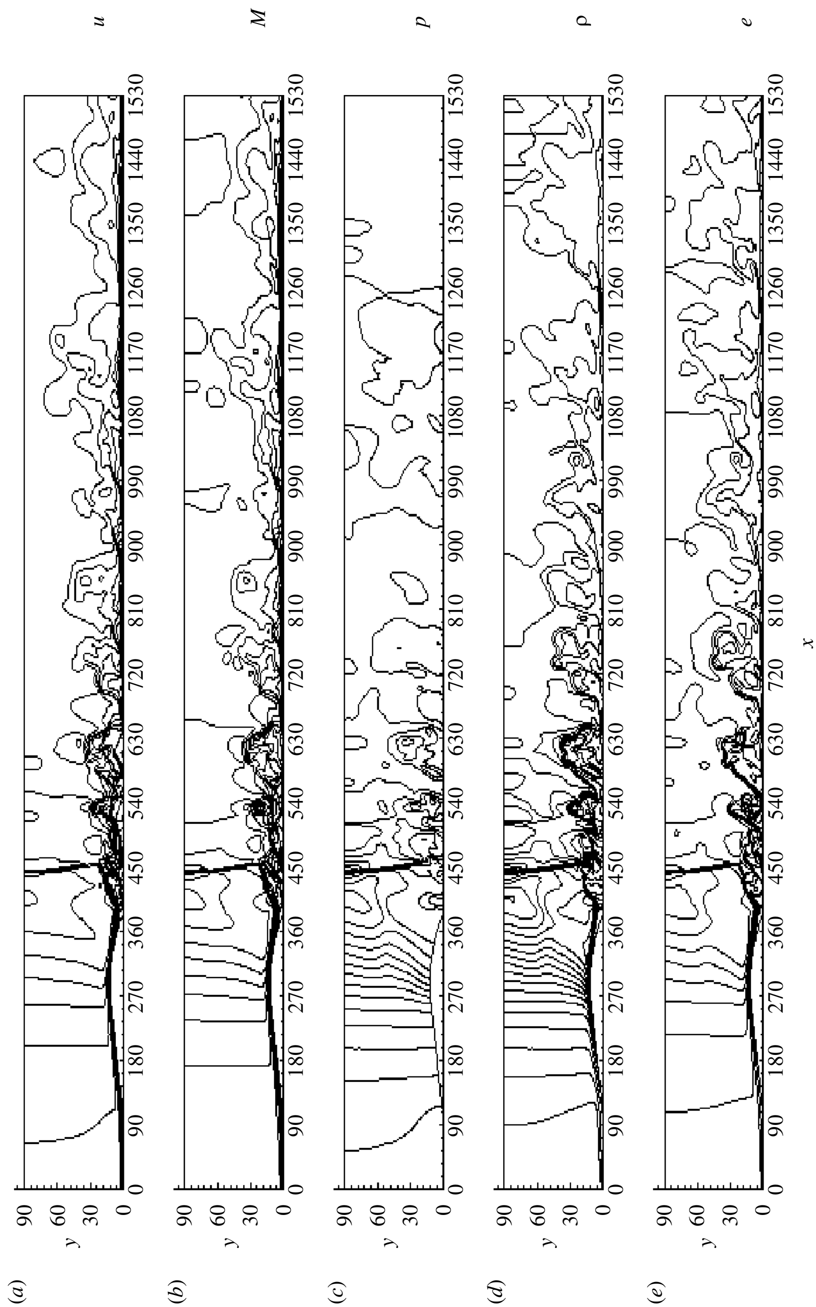

Figure 1. DNS of shock–boundary-layer interaction in transonic channel flow over a bump. The inlet Reynolds number is 1800 based on bump height. The computational grid size is $511 \times 101 \times 73$. Contours of velocity magnitude, Mach number, pressure, density and internal energy are shown. Figure courtesy of Professor N. D. Sandham, University of Southampton (UK Turbulence Consortium).

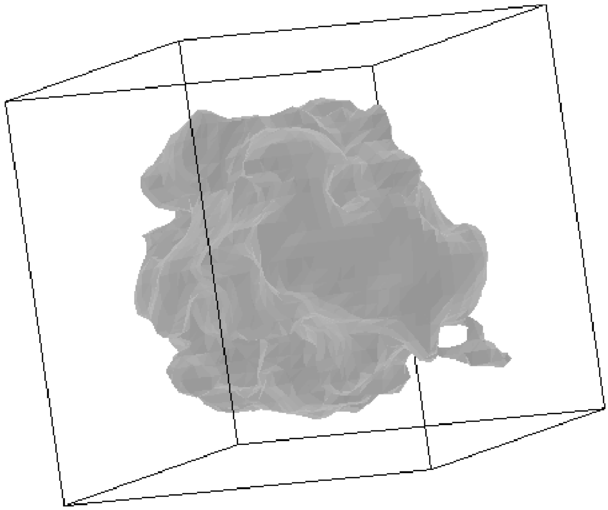

Figure 2. DNS of a turbulent flame kernel. The Reynolds number is 130 and the computational grid contains 384^3 (56.6 million) points. A surface of constant normalized reaction product mass fraction is shown. Figure courtesy of Dr K. W. Jenkins, University of Cambridge (via the Combustion Consortium).

is 150 based on the channel height, or 1800 based on the height of the bump. The computational challenge is to ensure adequate resolution of the turbulent boundary layer, particularly in the viscous region close to the wall, as well as to capture the location and strength of the shock wave. An entropy-splitting scheme was used together with a computational grid of $511 \times 101 \times 73$ (37.7 million) points. A three-dimensional simulation is essential in order to capture the evolution of the turbulence, and the computational domain has a spanwise width of 7.5 bump heights. Shock-wave–boundary-layer interactions of this type are of great importance in aircraft aerodynamics, where small changes in the shock location can produce large changes in the total drag, and where unsteadiness of the shock can lead to problems of aircraft stability. This class of DNS promises to offer new insight into the physics of the process.

In figure 2, results are shown for a DNS of a flame kernel growing through a turbulent fuel–air mixture (Jenkins & Cant 2001). The kernel is initially laminar and spherical, and the turbulence is initially homogeneous and isotropic. A surface of constant reaction product mass fraction is shown, and it is clear that the flame surface has become wrinkled and distorted by the embedding turbulence. A simplified chemical reaction mechanism has been employed, and the turbulence Reynolds number is 130. The computational grid contains 384^3 (56.6 million) points. This type of simulation is intended to provide fundamental data on flame–turbulence interaction over a curved flame surface, and to give some insight into the process of flame kernel growth which occurs for example in spark-ignition engines. Again, DNS is able to provide detailed information on quantities such as local hydrodynamic straining rates which are very difficult to measure experimentally.

3. Large-eddy simulation

The basis of LES is that as much as possible of the flow field should be resolved, leaving as little as possible to be modelled. This places LES in between the limiting cases of DNS and RANS. The computational requirements are similar to those of DNS, while the modelling requirements are similar to those of RANS. In practice, LES offers its own unique advantages. Unlike RANS, the accuracy of a well-formulated LES computation will approach that of DNS as the resolution improves. Furthermore, a great deal of local information is available at the grid scale in LES, which can be used to improve the accuracy of the sub-grid modelling. Since resolution is intended to be incomplete, it is unnecessary in LES to use DNS-like discretization schemes, and properly constructed schemes that have been developed for RANS are generally adequate.

There are many possible approaches to modelling the effects arising from the unresolved portion of the turbulence. A simple and remarkably successful strategy is to make the assumption that momentum and energy are dissipated by small-scale turbulence in a manner analogous to the effects of molecular viscosity. This approach was postulated by Smagorinsky (1963) and fits well with classical theories of turbulence. Nevertheless, in many circumstances of practical relevance, such as transitional boundary layers, there is transfer of momentum and energy from small scales to large scales, and this cannot be accounted for by a purely dissipative model. In order to overcome this difficulty, Germano *et al.* (1991) put forward the dynamic approach, in which the original LES filter is accompanied by a so-called 'test filter' at a length-scale that is somewhat larger. Differences in the observed sub-grid behaviour at the two separate filter scales are then used to infer the correct rate and direction of momentum and energy transfer. This general formulation can be used with Smagorinsky or other sub-grid models and has become a *de facto* standard for LES.

LES has proved especially appropriate for flows where there is large-scale unsteadiness, or appreciable levels of free-stream turbulence. Generally the method has proved less successful for near-wall flows, where the length-scales of turbulence decrease as the wall is approached. Adequate resolution of the key length-scales becomes increasingly difficult, and ultimately is impossible unless a DNS-like grid is adopted close to the surface. The alternative is to make use of near-wall models, but here LES offers little advantage over traditional RANS approaches. In combustion, the principal difficulty is in representing the structure of the flame, which in general is thin and falls well below the grid scale. Models for sub-grid mixing and reaction rate are now becoming available (Hawkes & Cant 2001). In due course, LES will have to be applied to complex industrial geometries and this poses new problems in terms of grid non-uniformity and lack of isotropy, and in terms of adequate resolution of both geometry and small-scale flow features.

Some examples of current practice in LES are shown in figures 3–5. Figure 3 shows contours of streamwise velocity in LES of an array of high-lift turbine blades from a low-pressure turbine in a typical modern jet engine. The flow is from left to right, and the blade row is rotating at a specified angular velocity relative to an upstream row of stator blades. The wakes leaving the exit boundary of the simulation are inverted, scaled and returned to the inlet to represent the incoming wakes. The simulation captures the effect of the wakes behind the stators as they impinge on the blades of

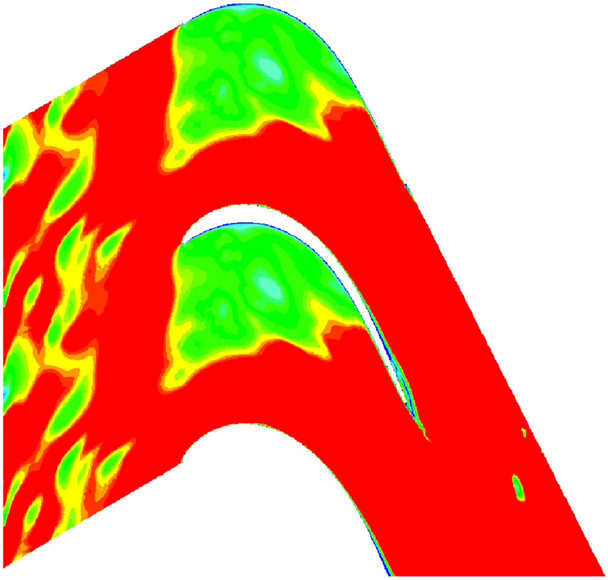

Figure 3. LES of rotor–stator interaction in a low-pressure turbine in a typical jet engine. Contours of streamwise velocity are shown. The flow is from left to right, and the blade row is rotating at a specified angular velocity. The wakes leaving the domain are rotated, scaled and returned to the inlet to represent the incoming wakes. Figure courtesy of Professor P. R. Voke, University of Surrey (LES-UK Consortium).

the rotor, causing significant changes in the local flow field and the lift pattern on the blades. This type of unsteady simulation cannot be performed adequately using RANS and requires the use of LES.

Figure 4 shows results from LES of a simplified geometry that represents the inlet section of a gas-turbine combustor (Tang *et al*. 2001). The flow from the compressor emerges from the left-hand boundary through a narrow passage into a larger plenum. There is a sudden change of area and the component is known as a dump diffuser. The problem has been tackled using a block-structured grid divided into four blocks, with a total of about 800 000 grid points in a small angular sector of the axisymmetric device. The grid structure is shown, together with mean streamlines and contours of instantaneous axial velocity. The inlet flow is turbulent and must be generated 'on the fly' using a precursor simulation upstream. It is clear that the instantaneous flow field contains many small features, and bears little more than a superficial resemblance to the mean picture. Indeed, the mean streamlines have been obtained by long-time integration of the simulation, and the collection of statistical data from LES in this manner is often costly. The advantage of LES in this case is that accurate prediction of the time-dependent flow field is essential in order to predict local rates of heat transfer from the combustor walls.

LES of a turbulent premixed flame is shown in figure 5. The flame is propagating downwards into an oncoming turbulent stream of combustible mixture, and the figure shows a surface of constant reaction product mass fraction (Hawkes & Cant 2001). Only the filtered flame is simulated, and hence there is a smoothing effect relative to the true flame surface. The sub-grid flame surface area is modelled using a

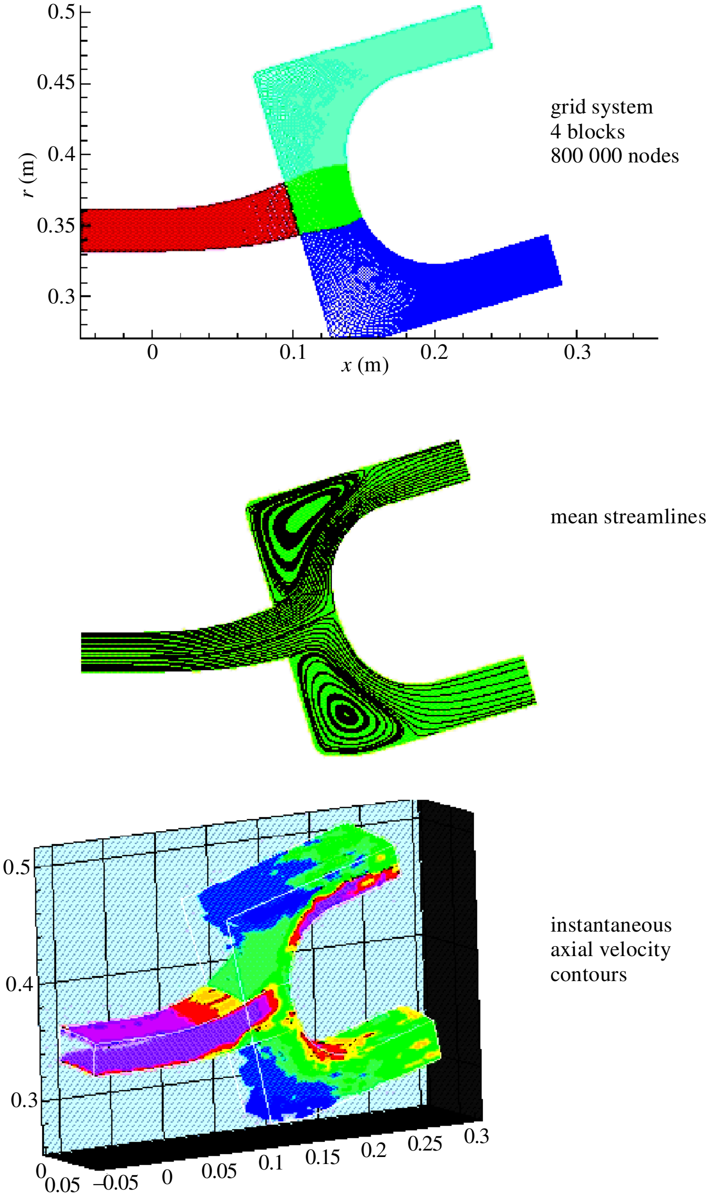

Figure 4. LES of flow in an axisymmetric dump diffuser geometry. The multiblock structured grid contains four blocks and a total of about 800 000 points. Inlet conditions are generated by a precursor simulation of the upstream channel flow. Contours of instantaneous axial velocity are shown together with mean stream lines obtained by long-time integration. Figure courtesy of Professor J. J. McGuirk, Loughborough University (LES-UK Consortium).

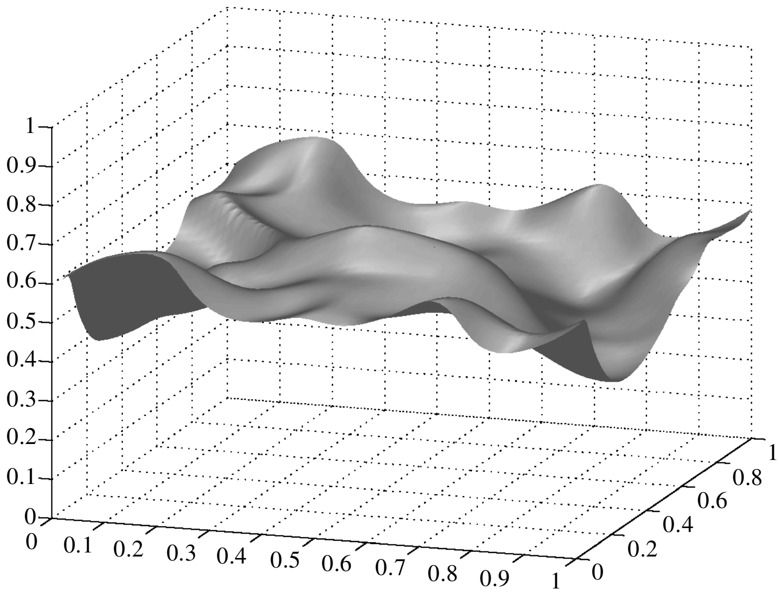

Figure 5. LES of a turbulent premixed flame. The sub-grid reaction rate is modelled using the flame surface density approach. The flame is propagating downwards, and a surface of constant filtered normalized reaction product mass fraction is shown. Figure courtesy of Dr E. R. Hawkes, University of Cambridge (via the Combustion Consortium).

transport equation for the flame surface density, with unclosed terms that are themselves modelled with guidance from DNS data. LES of such flames is necessary in order to capture large-scale unsteadiness which may be linked to acoustic instability in practical devices such as gas-turbine engines.

4. Reynolds-averaged Navier–Stokes simulation

As the power of computers continues to increase and LES is developed further it is clear that the importance of RANS will diminish with time. Nevertheless, for most industrial CFD tasks, RANS remains perfectly adequate. The approach is mature and its deficiencies are well understood. In many circumstances it is necessary to compute only the average behaviour of a system, there are often geometrical symmetries which an be exploited to reduce computational costs, and the flow is often statistically steady or two dimensional. In such a situation the additional computational cost of LES is simply not justified. A highly competitive commercial market now exists in off-the-shelf RANS-based CFD codes for industry.

A significant research effort continues in the development of new modelling capabilities for RANS, focusing mainly on the incorporation of new physics and on handling more complex problems. Significant research effort is also being expended in aspects of computational geometry (Dawes *et al.* 2001), which will help to make RANS, and in due course also LES, more applicable to complex industrial geometries. Research is also being carried out into the integration of RANS-based CFD into the engineering design process. Thus it is already possible to make use of 'virtual testbeds', where the effects of geometrical changes can be investigated computationally before metal is cut. The availability of HPC has not led to very large RANS computations. Instead, the standard k–ε and Reynolds stress turbulence models for RANS have benefitted indirectly from HPC through the availability of DNS data. RANS models for turbulent combustion have advanced significantly using data derived from DNS studies to validate modelling concepts as well as to refine the values of model constants.

An example of current RANS capability is shown in figures 6 and 7 (Birkby *et al*. 2000). Figure 6 shows contours of temperature on a cross-section taken through the centreline of a real industrial gas-turbine combustor geometry. Air is introduced into the combustor from a large enclosing plenum chamber (not shown) through an annular slot in the underside of the large disc structure seen in cross-section at the top. The air is divided into two streams which are driven into opposing swirling motion by a set of swirl vanes contained within the upper and lower air passages inside the disc. The location of the swirl vanes is indicated in the figure by the blank area in each air passage where the cutting plane has passed through the vanes. Natural gas fuel is introduced through a large number of small tubes located immediately downstream of the swirl vanes, and the fuel and air mix as the flow is swept down into the combustor barrel. At the bottom of the combustor there is a curved discharge nozzle leading to the high-pressure turbine. The overall length of the combustor is *ca.* 0.7 m, and the diameter of the fuel injector tubes is *ca.* 0.7 mm. Thus the range of length-scales in the geometry alone is approximately 1000:1. The geometry was supplied in CAD format, and following a process of geometry analysis and repair a surface mesh was generated. Detail of the triangular surface mesh is shown in figure 7 and serves to illustrate the degree of mesh refinement required for adequate resolution around the trailing edge of the swirl vanes and the exit from each of the fuel injector tubes. The unsteady RANS simulation was carried out on a three-dimensional unstructured tetrahedral mesh containing just under 500 000 tetrahedra, and the aim was to simulate the coupling between the unsteady flow, mixing and combustion at particular combustor operating conditions. Dynamic adaption of the grid based on the local solution was used near to the exit from each fuel injector tube in order to represent the details of the mixing process to a sufficient level of accuracy. The simulation succeeded in capturing the main characteristics of the device, and in identifying a potential source of combustion instability. This contributed to design changes which were adopted for subsequent production.

5. Challenges and conclusions

Progress in CFD as a result of HPC has been very significant but major challenges remain. The pattern of using HPC mainly for DNS and for research in LES is likely to continue, and the impact of DNS data in the development of new modelling is likely to increase. The major challenges facing DNS lie in the need to simulate ever more realistic and relevant problems. The attainable Reynolds number must increase in order to bring greater confidence in the scalability of DNS results. This implies that simulations must become larger in order to accommodate a greater range of scales. At the same time, better formulations for DNS boundary conditions are required so that more realistic simulations involving inflow and outflow can be tackled. In combustion DNS, the problems associated with accurate and efficient representations of complex chemical reaction mechanisms must be addressed. It is clear that turbulence scaling laws will ensure that DNS will be able to fill both the storage and computing capacity

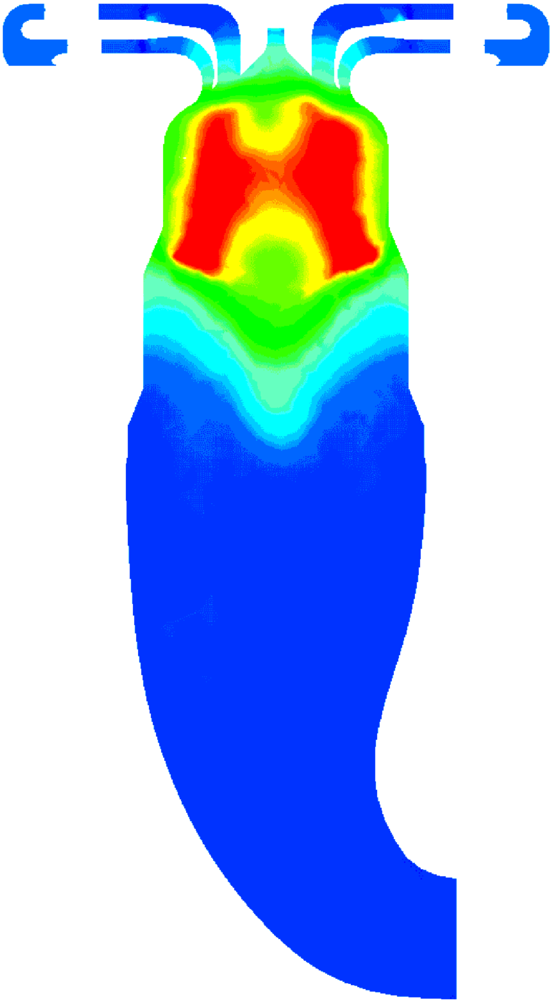

Figure 6. RANS simulation of flow and combustion in a real industrial gas-turbine combustor. Contours of temperature are shown. At this operating condition, combustion is taking place only in the primary zone close to the top of the combustor barrel. The unstructured tetrahedral grid for this simulation contains just under 500 000 tetrahedral cells.

of any projected HPC machine for many years to come. Thus there is a premium on the development of efficient algorithms and parallel computing strategies. Larger DNS means that output datasets will become larger, and there is a need for novel methods of dataset storage, annotation, analysis and visualization. It is clear that remote access to large distributed DNS datasets is an ideal task for the emerging GRID.

In the development of LES the main challenges lie in tackling realistic industrial problems. The use of multiblock or unstructured grids is likely to increase as new scale-independent models are developed. The difficulty in tackling wall boundaries must be addressed, possibly using novel wall-function treatments based on DNS data. In combustion, new models for sub-grid scalar transport and reaction must be

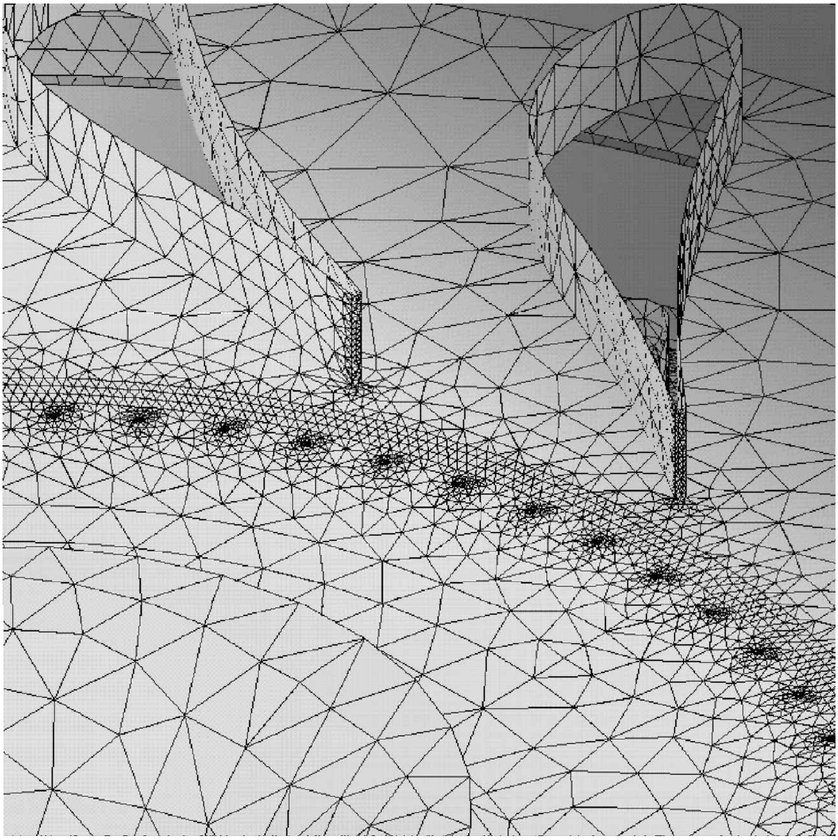

Figure 7. Geometrical detail showing the triangular surface mesh around the trailing edge of a number of swirl vanes and the exit from several fuel injector tubes in the industrial gas-turbine combustor. Each of the 128 tubes was *ca.* 0.7 mm in diameter, while the entire combustor was *ca.* 0.7 m in length.

developed to the point where they are both accurate and robust. Validation of LES results is a major area of concern, since it is rarely possible to obtain sufficiently detailed data from experiment, and the Reynolds numbers of available DNS data in general remain rather too small.

RANS will remain important for industrial simulations for the foreseeable future. Numerical methods, turbulence modelling and geometry handling in RANS are all well developed, but the possibility exists for further improvement in all of these areas. DNS data have already made a significant impact on RANS modelling, especially in the combustion area, and this is likely to continue. Future demands on RANS are likely to include much greater use of unsteady RANS approaches in order to achieve convergence with LES methods, and the use of RANS on problems with complex physics such as multiphase flow and biological fluid mechanics.

The importance of CFD in engineering is likely to increase still further as desktop computing power increases, while the accuracy of desktop CFD is likely to increase considerably thanks to developments in DNS and LES. The possibility still exists of a breakthrough in fundamental understanding of turbulence, and this may yet come using research tools based on DNS. That remains the greatest challenge of all.

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