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Numerical Simulation of the Dynamics of Turbulent Boundary Layers: Perspectives of a Transition Simulator

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Numerical simulation of the dynamics of turbulent boundary layers: perspectives of a transition simulator

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The current and prospective capabilities of numerical simulations of turbulent boundary layers are discussed. The stringent resolution requirements for resolving instantaneous structures and dynamics (rather than just for producing statistics) are emphasized. Improvements and alternatives to the prevailing simulation methodology are proposed.

1. Introduction

Numerical simulations of turbulent boundary layers in shear flows established their credentials as a productive research tool in the 1980s. Naturally, many of the early efforts concentrated on establishing the credibility of simulations by reproducing the mean flow and low-order turbulence statistics of highly idealized flows. However, as has been summarized recently by Reynolds (1990), the unique product of simulations – information on the complete space-time flow field – has been exploited in a number of investigations to reveal new insights into turbulent flow. Nevertheless, numerical simulations have been reported to date only for extremely simple geometries – channels and flat-plate boundary layers – under the assumption of periodicity in the streamwise and spanwise directions and at low Reynolds number. This limited range of applications has been due partly to the constraints on what can be computed reliably with existing algorithms on current computers and partly to difficulties in formulating problems in more complex geometries.

In the present article we discuss the prospects for numerical simulations of turbulent boundary layers in the coming years, with a particular emphasis on their role in unravelling structure and dynamics. The reader is advised that the author's own expertise is on transitional flow rather than turbulent flow and is making his remarks as a casual participant in the field.

2. Current DNS and LES capability

In some quarters the term 'numerical simulation' is taken to encompass just direct numerical simulation and large-eddy simulation. Direct numerical simulation (DNS) involves the numerical solution of the full nonlinear, three-dimensional, time-dependent, Navier–Stokes equations for prescribed initial and boundary conditions without any empirical closure assumptions. The numerical methods used for this purpose are very similar to those which are used for simulations of transition; see Kleiser & Zang (1991) for a recent review of this related subject. Large-eddy simulation (LES) uses a 'subgrid-scale' model for those length scales which are too

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small for the computational grid to resolve. The article by Reynolds (1990) (and the companion articles in that volume) as well as the proceedings of a recent conference on LES (Galperin 1991) furnish a current survey of the field.

DNS of turbulent flows requires enormous computer resources. High-fidelity simulations of turbulent channel flow have been published for a Reynolds number, Re, of 3300 (based on channel half-width and mean centreline velocity) by Kim *et al.* (1987) and at $Re = 3800$ by Gilbert & Kleiser (1988). Preliminary results for an on-going computation by the present author at $Re = 6200$ were reported in Zang *et al.* (1990). The grid spacings in the streamwise and spanwise directions for these three simulations were, to within 20%, $\Delta x^+ \approx 10$ and $\Delta z^+ \approx 6$; the first grid-point away from the wall was at $y^+ \approx 0.06$, and there were a dozen grid points between the wall and $y^+ = 10$. (Dimensions are given in wall units, for which the velocity, length scales and timescales are, respectively, $u_\tau = \sqrt{(\nu\, \partial\bar{u}/\partial y)}$, $l_w = \nu/u_\tau$, and $t_w = \nu/u_\tau^2$, where ν is the kinematic viscosity.) The lengths of the computational domains in the periodic streamwise and spanwise directions were typically $L_x^+ \approx 2000$ and $L_z^+ \approx 1200$. A DNS of a turbulent boundary layer with a Reynolds number based on momentum thickness of $Re_\theta = 670$ was performed by Spalart (1988) and later repeated at finer resolution by Robinson *et al.* (1989). The resolution and domain size of the latter calculation were comparable with those of the channel flow simulations except for the streamwise direction, in which the grid spacing and the domain size were twice as large as for the typical channel flow case. (Most of these simulations utilized some form of de-aliasing; the grid spacings cited above pertain to the smallest scales which were fully captured.) These direct simulations used on the order of 10^6–10^7 grid points. The computations were run for about 1000 t_w and took several hundred CPU hours.

The resolutions used for the high-fidelity DNS cited above appear to have been guided by statistical considerations, such as producing, for the prescribed Reynolds number, correct (1) mean flows (judged by the accepted logarithmic layer), (2) root-mean-square velocity fluctuations, (3) spanwise spacing of the low-speed streaks, and (4) skewness and flatness statistics. The latter requirement is the most stringent and evidently requires horizontal one-dimensional energy spectra which decay by at least three orders of magnitude. (We should note that even low-fidelity simulations can produce a mean flow which has a turbulent shape; however, inadequate resolution usually results in a mean flow appropriate for quite a different Reynolds number.) There appear to be little published information which establishes quantitatively the level of numerical error in the few high-fidelity DNS which are available. (However, Rai & Moin (1989) do compare the turbulence statistics of the Kim *et al.* (1987) channel flow computation with those obtained on two grids with a different numerical method.)

Medium-fidelity simulations, such as are typically furnished via LES, achieve criteria (1), (2) and perhaps (3). According to current practice (Piomelli *et al.* 1988; Yakhot *et al.* 1989), the resolution requirements for LES appear to be $\Delta x^+ \approx 80$, $\Delta z^+ \approx 30$, with the first grid-point off the wall at $y^+ \approx 2$ and approximately three points between the wall and $y^+ = 10$. Such simulations have barely enough resolution to resolve the wall streaks and the sweep and ejection events; nevertheless, even though these structures are somewhat diffused by the model and the coarse grid, the low-order statistics are acceptable. At Reynolds numbers comparable with those of the DNS cited, LES utilize on the order of 10^5 grid-points and take a few CPU hours. Of course, LES utilizing more grid-points can be used to reach higher Reynolds

numbers, perhaps by as much as a factor of 5 over DNS, if one expends 10–100 CPU hours. This relatively low cost of the LES has permitted some grid-refinement studies to be conducted (Piomelli *et al.* 1988).

Although present subgrid-scale models are still primarily of the algebraic eddy viscosity type, there have been some promising recent developments, such as renormalization group models (Yakhot *et al.* 1989) and dynamic eddy viscosity models (Germano *et al.* 1991) that remove the *ad hoc* modifications to the basic Smagorinsky subgrid-scale model that were formerly used in the near-wall region (Moin & Kim 1982). Curiously, relatively little attention has been paid to what is gained from the subgrid-scale model over simply performing a DNS on the same, coarse grid as used for the LES. The simulations of Piomelli & Zang (1991) are an exception to this, and their channel flow computations do indicate that LES results are indeed superior in terms of criteria (1) and (2) to those of coarse-grid DNS.

The ability of DNS and some LES to produce the known statistical properties of turbulent boundary layers has lent confidence to the use of this type of numerical data for extracting the dominant coherent structures in turbulent flows. An oft-repeated motivation for this type of work is that knowledge of the important structures will facilitate understanding of the dynamics of turbulence and that, in turn, can lead to improved methods for turbulence control and to improved Reynolds-averaged turbulence models. The most elaborate study of this type was undertaken by Robinson (see Robinson *et al.* 1989). Some of the significant structures that he catalogued included; quasi-streamwise vortices (primarily one-sided), near-wall shear layers, and horseshoe vortices. The typical scales of these structures were as small as $30l_w$ in z (for the quasi-streamwise vortices and the near-wall shear layers) and as large as $500l_w$ in x (for the near-wall shear layers).

The conclusions drawn from current DNS results about the presence of these structures and their length scales are certainly reliable, whereas LES represent these structures crudely at best. However, at present one must maintain a healthy skepticism about whether even DNS of low Reynolds flows at current high-fidelity levels can capture reliably the instantaneous shapes and dynamics of turbulent structures.

Resolution levels comparable with those used for turbulent flow DNS have proven inadequate to capture reliably similar vortical structures in transitional flows. (Among others, Wallace (1982) has observed a strong similarity between the vortices found in the early non-linear stages of transition and those in turbulent boundary layers.) For example, fig. 15 of Robinson *et al.* (1989) displays a horseshoe vortex on which a secondary vortex has emerged (similar to the structures found experimentally by Smith (1984)). This object has dimensions of $400l_w$ in x and $140l_w$ in z and it was computed with approximately 12 points in x and 20 points in z. Zang *et al.* (1989) simulated the transitional equivalent of such a structure at various levels of spanwise resolution (while ensuring adequate resolution in the other two directions). Figs 10–14 of that paper demonstrate that there are significant differences in the evolution of the vortical structure as computed with 8, 12, 16, and even 32 points in z compared with an ultra-fidelity computation using 324 points in z. For the 8-point (in z) case the horseshoe vortex evolved far too slowly, to the point that a secondary vortex never quite materialized, whereas for the 12, 16 and even the 32-point cases it evolved too rapidly and was contaminated with serious errors in the vicinity of the secondary vortex and at the wall just upstream of the vortex tip.

These results suggest that reliable computation of the dynamics of near-wall

turbulent structures will demand an increase in the resolution presently customary for turbulence simulations by at least a factor of 2 and perhaps by an order of magnitude. One must also bear in mind that the traditional time-differencing schemes (Adams–Bashforth and Runge–Kutta) become increasingly inaccurate at the smaller scales.

In view of the likelihood that the detailed dynamics of what is captured in high-fidelity DNS are unreliable and yet the simulations nevertheless capture even fourth-order statistics quite well, one must wonder about the importance of these fine details to the turbulence. Of course, the detailed dynamics may turn out to be much more significant at higher Reynolds numbers.

3. Improved simulation algorithms

When one compounds the need for higher resolution with the desire to escape from the low Reynolds number régime to which present DNS and LES are confined, the need for improved simulation methodology is apparent. The drastic increase in computer requirements as the Reynolds number is increased is well known, with the requisite number of grid-points scaling as $Re^{\frac{3}{4}}$ in each coordinate direction. The upper limit of the computer time that research laboratories have historically made available to a single DNS computation is about 2% of the CPU hours available for an entire year on the local supercomputer. At present such laboratories typically have an 8-processor Cray YMP, which is capable of sustaining slightly more than 10^9 floating-point operations per second (FLOPS) on a simulation code. Even if the fond hopes of achieving sustained speeds approaching 10^{12} FLOPS by the year 2000 are realized, we can expect out of present DNS algorithms at most ultra-fidelity (dynamical) resolution levels (factor of at least 4 in each direction) at current Reynolds numbers or high-fidelity (statistical) resolution levels at Reynolds numbers a factor of 5 larger.

There are clearly algorithmic improvements that can be made to alleviate the computational burden of conducting DNS with the added resolution necessary to investigate dynamics or to get to higher Reynolds numbers. Foremost among these is to replace the current workhorse methods which are based on the eulerian (as opposed to the lagrangian) framework and which depend upon global, tensor product grids with domain decomposition methods. These methods would facilitate not only local refinements (including time-dependent grid adaptation), but also simulations in more complex geometries. Local refinements would be particularly helpful for the wall layer, since the spanwise resolution required beyond, say $y^+ = 30$, is much less demanding. They would also help in simulations of spatially developing turbulence for which there are local regions, such as separation zones, which require fine grids. Improved time-differencing schemes are also needed (see Kleiser & Zang 1991).

The historical preference in the numerical simulation community for global grids has been due primarily to the availability of fast, direct methods for solving the implicit equations that arise in DNS algorithms (especially ones for incompressible flow) and the relative inefficiency of iterative solution schemes. The balance is now shifting in favour of the latter. Multigrid methods (cf. Mandel *et al.* 1989) have recently become competitive with direct methods for three-dimensional problems on global grids and they suffer little degradation in efficiency when local refinements are used.

The forthcoming methods of choice are likely to be finite-difference/finite-element methods of fourth- or sixth-order accuracy and spectral domain de-

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composition methods. (See also the alternative methods discussed below.) With the former methods the requisite local grid spacing is two-thirds of that cited above for spectral methods. Comparisons between spectral and high-order finite-difference methods made on the basis of statistical criteria are surely over optimistic about the accuracy of finite-difference methods on instantaneous dynamics.

Finally, let us mention that simulations of true, spatially developing turbulence are on the horizon. One of the critical needs here is for means to specify turbulent inflow conditions in a realistic manner.

4. Adulterated numerical simulation

In the words of Aubry *et al.* (1988) one of the more ambitious goals of research into turbulent boundary layers is to 'dismantle the system and show ... how it works.' This involves more than reproducing the statistics of turbulent flow or even identifying the dominant structures, although these are necessary first steps.

The remarks quoted above were made in the context of motivating numerical computations of turbulent flow with a low-order dynamical system comprised of the most energetic coherent structures. Numerical simulations can be exploited in a complementary fashion. There are a variety of ways in which this can be accomplished. Perhaps the most straightforward to implement is to modify the contributions made by specific terms in the Navier–Stokes equations in all or selected regions of the flow. One can also suppress or enhance the presence of coherent structures, whether treated as waves (Aubry *et al.* 1988; Sirovich *et al.* 1990) or as local eddies (Moin & Moser 1989). This might proceed by using DNS data to identify the structures (as in the preceding two references), then to perform a computation in which the contribution of specified structures is identified at every step and altered as desired. This would provide more direct evidence for the dynamical significance of the structure than simply correlating it with, say, Reynolds stress. At yet another level one might attempt to interfere with feedback loops. For example, there is speculation that an important component to turbulence regeneration is the creation of vorticity at the wall by the pressure field associated with horseshoe/hairpin vortices (Walker 1990). Why not alter this component of the pressure and see what happens?

This approach might be termed *adulterated* numerical simulation. It has seen some use in transition simulations (see, for example, the effects of suppressing streamwise vortices reported by Krist & Zang (1989)) but has gone virtually untapped in turbulence simulations.

5. Alternative methods

Despite the substantial achievements of conventional numerical simulations during the 1980s, it is surely time to devote comparable computer resources to alternative simulation tools, such as vortex methods, lagrangian schemes, and asymptotic approaches.

DNS (or even for some purposes LES) can be used to identify the essential structures of turbulent flow while their dynamics and high Reynolds number behaviour can be studied by other means. Here we wish to focus on the asymptotic approaches and merely mention Hon & Walker (1991) and Cowley *et al.* (1990) as recent applications of vortex and lagrangian methods, respectively, that offer clear advantages over DNS for high Reynolds number effects.

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Perhaps the asymptotic methods that have become so advanced, first for laminar, separated flows, then for transitional flows, and are just now beginning to be applied in a very qualitative manner to turbulent flows (Walker 1990; Smith *et al.* 1990) can be profitably adapted to what might be termed rational numerical simulations (RNS) of turbulent régimes. This approach yields different sets of partial differential equations in several 'domains' of the flow. In the near-wall region they have most of the complexity of the full Navier–Stokes equations and they can be solved by techniques similar to those used in conventional DNS (see, for example, Duck 1990). The equations in other domains often have an inviscid character and may best be tackled by vortex or lagrangian approaches.

There are potential difficulties with the well-posedness of the RNS equations; for example, they appear to admit finite-time singularities. It would be fruitful to interest the mathematical and numerical analysis communities in them. Investigations have already begun for problems which link the Navier–Stokes equations in the near-wall region with the Euler equations in the wake (Gastaldi & Quarteroni 1989; Quarteroni & Valli 1990). Given the success of numerical analysts during the 1980s in providing not only a rigorous justification for many of the algorithms used in DNS but also in devising useful new methods (see Canuto *et al.* 1988), there is reason to hope for clarification from these quarters. Another issue is how to configure algorithms which permit strong interactions (usually through transport of vorticity) from one region to another (see, for example, Peridier & Walker 1989).

Serious consideration should be given to establishing the credentials of RNS. The obvious starting point is a problem from the cleaner realm of transitional flows. To cite just one example of an application to a transition problem, Hall & Smith (1991) have developed a vortex–wave interaction theory (VWIT) for the strongly nonlinear interaction between streamwise vortices and travelling waves. There remains considerable controversy within the transition community as to the validity of this approach, with a quantitative verification of VWIT still lacking from either experimental or DNS data. It is surely feasible to conduct such a comparison between DNS and RNS based on VWIT for a transition problem and to evaluate the asymptotic approach. The next step would be to compare the predictions of DNS and RNS for turbulent channel flow.

Yet another approach from the transition community is worth considering. Bertolotti and Herbert (see Bertolotti 1990) have developed an economical methodology for treating spatially developing transition problems based on the parabolized stability equations (the PSE method). While perhaps lacking the formal mathematical basis of strongly nonlinear asymptotics, the PSE method has produced remarkable quantitative agreement at finite Reynolds numbers with both experiment and DNS. Bertolotti's results agree very well, for example, with the DNS results of Fasel *et al.* (1990) for ribbon-induced transition up to the laminar breakdown stage. The PSE results were obtained in minutes on a Cray YMP compared with hundreds of hours for the DNS results. There seems no reason why the PSE system cannot be extended to a 'parabolized turbulence equations' (PTE) system (by including far more temporal frequencies in the system). The PTE may turn out to be an economical means of studying spatially developing turbulence, although their relative advantage will be less than it is for transitional flows due to the need to include many more temporal frequencies.

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6. Concluding remarks

The challenges for numerical simulations include elucidation of turbulence dynamics rather than just statistics or even kinematics, application to flows at higher Reynolds number, and simulation of flows in more complicated geometries. These challenges are likely to be met in a variety of ways. Some progress can be made by increased computational power and improved DNS algorithms. However, novel approaches, such as adulterated numerical simulation, rational numerical simulation and parabolized turbulence equations are worthy of trial.

In addition to references specifically cited below, the author's opinions on this subject have been influenced by remarks made at several recent workshops by J. Ferziger, J. Kim and U. Piomelli and by the comments of the editor.

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