Direct Numerical Simulation of Turbulent Flows

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April 26, 1999

Abstract

Direct numerical simulation (DNS) of turbulent flows is reviewed here. Background of DNS is presented and the importance of DNS in turbulence is highlighted. Further, we discuss related numerical issues such as the available methods, boundary conditions and spatial and temporal discretizations. Finally, impact of DNS on turbulence modeling is described and the future possibilities of this tool are contemplated.

1 Introduction

The complex behavior of turbulence is the consequence of a fairly simple set of equations - the Navier-Stokes equations. However, analytical solutions to even the simplest turbulent flows do not exist. A complete turbulent flow, where the flow variables like velocity and pressure are known as a function of space and time can therefore only be obtained by numerically solving the Navier-Stokes equations. These numerical solutions are termed as Direct Numerical Simulations (DNS) [10]. The main purpose of DNS is to solve (to best of our ability) for the turbulent velocity field without the use of "turbulent modeling". This condition means that the Navier-Stokes momentum equation for fluid must be solved exactly, which is not a simple task. Turbulence modeling involves the estimation of the increased fluid stresses due to the swirling motion of a turbulent flow field. Before the advent of powerful supercomputers, the effect of high-frequency velocity fluctuations within a flow field was estimated using modeling techniques, resulting in a macro-scale, or an integral-sense of the flow properties. Nowadays, the Navier-Stokes equation can be solved directly through the use of fast, large memory capacity computers using highly specialized numerical techniques, i.e. we can now examine fully developed turbulence flow fields at a micro-scale and perform extremely accurate calculations of flow properties. For the discretization, relatively fine grid sizes are necessary. Thus, any DNS code is very time consuming and has extensive storage requirements. Until now, only DNS computations at moderate Reynolds numbers are possible.

DNS using high-performance computers is an economical and mathematically appealing tool for study of fluid flows with simple boundaries which become turbulent. DNS is used to compute fully nonlinear solutions of the Navier-Stokes equations which capture important phenomena in the process of transition, as well as turbulence itself. DNS can be used to compute a specific fluid flow state. It can also be used to compute the transient evolution that occurs between one state and another. DNS is mathematical, and therefore, can be used to create simplified situations that are not possible in an experimental facility, and can be used to isolate specific phenomena in the transition process. As we are aiming at a nearly exact solution (and not “the” exact) to specific turbulent flows utilizing limited computational resources, DNS is stressed as a research tool and not as a brute-force solution. The objective of DNS is not necessarily to reproduce real-life flows (say the flow over an airplane), but to perform controlled studies that allow better insight, scaling laws, and turbulent models to develop. In aerodynamics, DNS is associated with a large-scale computationally intensive solution procedure which may consume hundreds to thousands of Cray Super-computing resources. The earliest use of DNS began in the 1970’s and with the growth in the computational power today, it is getting more and more popular day by day [4]. Current computations typically use finite-difference schemes, or a combination of spectral and finite-difference schemes, although finite element approaches using unstructured grids are also being explored.

However, the main technical challenges of DNS remains the memory and computational speed requirements. A DNS of the flow past a complete airfoil would require a computer with exaflop (10^{18} flops) capacity to be practical, which is still not available now. The instantaneous range of scales in turbulent flows increases rapidly with the Reynolds number and hence most practical engineering problems (e.g. flow around a car) have too wide a range of scales to be directly computed using DNS. The difficulty in the DNS is that the turbulence contains wide spectrum of vortices with an equal physical importance. With increase of the Reynolds number, the size ratio of the largest to the smallest vortices increases. This makes it difficult to perform the DNS of turbulence with a higher Reynolds number. Thus for most high Reynolds number applications today, approximations like Large Eddy Simulation (LES) which computes only the large energy-containing scales, and Reynolds averaged Navier-Stokes solutions (RANS) are more prevalent than DNS. DNS can be thought of as the most desirable solution to a turbulent flow problem which is much more computationally intensive, followed by LES which is less complex and then RANS which is the least complex (and also the coarsest approximation).

2 Background

The foundations of DNS were laid at the National Center for Atmospheric Research in 1972 by Orszag & Patterson [12], who used spectral methods to perform a 32^3 computation of isotropic turbulence at a Reynolds number of 35 (based on Taylor microscale).

The next major step was taken by Rogallo [15] in 1981, who combined a transformation of the governing equations with an extension of the Orszag-Patterson algorithm to compute homogeneous turbulence subjected to mean strain. The results were compared to theory and experimental data and used to evaluate several turbulence models which set the standard for DNS of homogeneous turbulence. The earliest computed flows were inhomogeneous in only one direction. The computing resources in the late 1970's did not allow DNS of wall-bounded turbulence; however, coarse-grid computations of free-shear layers could be performed. It was not until 1987 that the DNS of the plane channel flow was performed [6]. The next major step was taken by Spalart [16], who developed an ingenious method to compute the turbulent flat-plate boundary layer under zero and favorable pressure gradients. Computing flows that are inhomogeneous in the streamwise direction required that the turbulence be specified at the inflow plane. A recent advance has been the development of methods to specify this inflow turbulence, as a result of which reasonably complex flows, e.g. the flow over a backstep (Le & Moin [7] in 1994), and flat plate boundary layer separation (Na & Moin [11] in 1996) have been computed.

In contrast to its incompressible counterpart, DNS of compressible turbulent flow has been fairly recent. The DNS of homogeneous compressible turbulence was initiated in 1981 by Feiereisen *et al.* [3], but a serious study of compressible homogeneous turbulence (isotropic and sheared) was undertaken only a decade later. Wall-bounded flows such as the compressible channel and turbulent boundary layer have only recently been attempted. Recently, DNS has also examined high-speed turbulent mixing layers and the interaction of shock waves with turbulence. An exciting new development has been the field of computational aeroacoustics, where both the fluid motion and the sound it radiates are directly computed using DNS.

In tracing the evolution of DNS over the past decade, it is observed that the complexity of the computed flows has noticeably increased, but that their Reynolds number is still low. Another development has been the increased investigation of turbulence physics by computing idealized flows that cannot easily be produced in the laboratory. As the geometry of the flows has evolved, so have the numerical methods. These changes have been accompanied by a significant improvement in computer hardware. Currently available parallel machines like the 64 processor SP-2 are about 100 times faster than the 64 processor ILLIAC-IV used in the early 1980s.

3 Numerical Issues

While speed increases brought by faster computer goes significantly to what can be accomplished using DNS, smarter programming, faster algorithms and novel theoretical tools receive continued emphasis to make progress in DNS.

For periodically assumed flows, fast Fourier series methods have enabled numerous temporal DNS studies. For the spatial DNS approach, high order ($\geq$ 4th) finite difference methods are commonly used in DNS codes. Due to the advances made by Lele [8], high-order compact difference techniques have been included in more recent DNS efforts. Spectral element and collocation methods have been used for spatial discretization around complex geometries [2]. Chebyshev collocation techniques (which use polynomials instead of trigonometric terms and are hence for non-periodic flows) have been used in boundary-layer and channel flow problems. Also, numerous DNS studies have used schemes like Adam-Bashforth, Runge-Kutta, Crank-Nicolson, and time-splitting approaches for time advancement.

Often Poisson or Helmholtz equations (Dirichlet and Neumann boundary conditions) must be solved during the course of a DNS. A Gauss-Siedel like iteration procedure and direct solvers have been used in DNS codes for these. Fast serial and parallel high-order direct solvers for Poisson and Helmholtz equations have been tested for speed and accuracy.

3.1 Spectral Methods

The major problem with any numerical solution of a differential equation is accurate calculations of derivatives. This is why nearly all early turbulence DNS's utilized spectral methods, which are extremely accurate and non-dissipative tools for calculating derivatives of discrete data sets. If crafted correctly, such methods enjoy exponential convergence to a highly accurate solution. A spectral method actually approximates a real-space function with a series sum of orthogonal functions. Mathematically, this looks like:

$$f(x_j) = \sum_{n=0}^{N-1} \hat{f}_n \phi_{n,j} \qquad j = \{0, 1, \cdots, N-1\} \tag{1}$$

The most common choice for the orthogonal functions is the Fourier series. This may seem to complicating things, but actually this helps to calculate the spatial derivative of f since Fourier series functions (complex exponentials) are easy to differentiate. Again, mathematically this results in:

$$f_j = \sum_{n=0}^{N-1} \hat{f}_n e^{i\omega_n j} \qquad \& \qquad f_j = \frac{1}{N} \sum_{n=0}^{N-1} \hat{f}_n e^{-i\omega_n j} \tag{2}$$

which are the inverse Fourier transformation and the Fourier transformation, respectively. Now, we can differentiate f :

$$\frac{\partial f}{\partial x_j} = \sum_{n=0}^{N-1} \underbrace{i\omega_n \hat{f}_n}_{\hat{g}_n} e^{i\omega_n j} \tag{3}$$

Therefore, in order to calculate the derivative of f, (1) calculate the Fourier transform, (2) compute new Fourier coefficients, and (3) calculate the inverse Fourier transform of the new series (with calculated coefficients from (2)). This method is quite time consuming, but with the help of the Fast Fourier Transforms (FFT), the method becomes $O(N \log N)$ instead of $O(N^2)$. However, several important stipulations must be observed when using this method to solve the Navier-Stokes equation:

1. The orthogonal functions should be well behaved and continuous to reduce Gibb's phenomena as much as possible (i.e. to recover pointwise exponential accuracy at all points including the discontinuities).

2. Grid spacing must be on the order of the Kolmogorov scale of the flow (smallest scale within the flow).

3. Aliasing errors (false translation of new modes into the domain) due to convective terms should be removed. They can cause either numerical instability or excessive turbulence decay.

One of the big disadvantages of this method is that it is not yet clear how these procedures can be extended to curvilinear grids which is so common in aerodynamics.

3.2 Finite Difference *vs.* Spectral Methods

In a comparative study, Rai & Moin [14] examined the influence of a finite difference *vs.* a spectral approach on the statistical results by comparing the turbulence statistics of their earlier computations using spectral methods (Kim *et al.* [6]) with those obtained using various finite difference techniques. They concluded that the prevalent method for DNS of turbulent flows is the spectral method, but that for complex geometries, finite difference techniques, especially high-order accurate upwind-biased methods, are good candidates. The statistical results obtained from the finite difference computations showed a reasonable but not excellent agreement with the results obtained earlier with the spectral method. However this is not sufficient to justify a conclusion on the performance of finite difference schemes, as the total number of grid points used for the finite difference computations was just 35% of those used for the spectral method.

3.3 Spatial Resolution

The range of scales that need to be accurately represented in a computation is dictated by the physics. The grid determines the scales that are represented, while the accuracy with which these scales are represented is determined by the numerical method. The Kolmogorov length scale, $\eta = (\nu^3/\varepsilon)^{1/4}$, is commonly quoted as the smallest scale that needs to be resolved. However, this requirement seems to be too stringent, and it is observed that the smallest resolved length scale is required to be of $O(\eta)$ and not equal to η. Spectral DNS shows very good agreement with experiments even though the Kolmogorov scale is not resolved. The smallest length scale that must be accurately resolved depends on the energy spectrum, and is typically greater than the Kolmogorov length scale; e.g. Moser & Moin [6] noted that most of the dissipation in the curved channel occurs at scales greater than 15η (based on average dissipation).

The resolution requirements are also fairly influenced by the numerical method used. Differencing schemes with larger numerical error would require higher resolution to achieve the same degree of accuracy compared to the spectral methods and the other more accurate finite differencing counterparts. Other factors which influence the spatial resolution are the differentiation error and the errors associated with the nonlinearity of the governing equations (triadic interaction between the scales, and aliasing), which should be sufficiently small.

And then of course, the Reynolds number plays the most important role. An acknowledged limitation of DNS is its restriction (by cost considerations) to low Reynolds number. For channel flow, the approximate number of grid points needed can be estimated from the expression by Wilcox [17]

$$N_{DNS} = (0.088\mathrm{Re}_h)^{9/4}$$

where Re_h is the Reynolds number based on the mean channel velocity and channel height. According to the above expression, to compute a flow with Reynolds number of 10^6 which we encounter in real-life, we would require approximately 133 billion grid points which is astronomical. To reduce this cost somewhat, Reynolds number scaling is used whenever possible depending on the observed dependence of the flow on the Reynolds number without changing the essential physics. Thus the choice of optimum Reynolds number for DNS is dependent on the application, as DNS need not obtain real-life Reynolds numbers to be useful in the study of real-life applications.

3.4 Temporal resolution

A wide range of time scales puts turbulent flows into the category of stiff systems for time advancement. Such stiff systems are often handled using implicit time advancement algorithms in CFD which allow use of large timesteps. Unfortunately, the requirement of time accuracy over a wide range of scales does not permit very large timesteps in DNS. Use of large timesteps implies that the small scales can have large errors, which can corrupt the solution. A common practice in incompressible DNS of wall-bounded flows is to use implicit time advancement for the viscous terms and explicit time advancement for the convective terms. For DNS of turbulent channel flow using implicit timestepping, studies by Choi & Moin [1] showed that very large timesteps cause the turbulence to decay to a laminar state.

3.5 Boundary Conditions

Boundary conditions have always been a critical issue in the use of DNS. Specifying boundary conditions at open boundaries is a difficult issue. For incompressible flows, statistically homogeneous directions such as the spanwise direction in a 2-D boundary layer are straightforward to treat and periodic conditions are imposed. However, most fully developed complex flows are inhomogeneous in the streamwise direction, which require both inflow and outflow boundary conditions to be specified.

Compressibility introduces additional boundary condition issues. Characteristic analysis must be used in compressible DNS to determine the number of boundary conditions required.

In the far-field, disturbances are generally assumed to vanish, so either homogeneous Dirichlet or exponentially decaying boundary conditions have been used. But these assumptions can lead to considerable errors when the nonlinear effects are large and the mean-flow distortion quantity is important.

4 DNS and Experiments

DNS results have consistently shown excellent comparisons with experimental data. One of the comparisons of the results obtained by DNS of turbulent flow over a backward-facing step (Le *et al.* [7]) with the experimental data obtained by by Jovic & Driver [5] is shown in figure 1. In 1987, Moin & Spalart [9] used DNS data from a turbulent boundary layer to estimate the accuracy of cross-wire probes and to quantify the magnitudes of the different sources of error. DNS has recently been used to provide probe design criteria and validate experimental measurements of vorticity in turbulent flows. Kim *et al.* [6] performed DNS of the turbulent channel flow ($Re_c = 3300$) using about 4 million grid points to resolve the flow. Extensive comparison of the results to experimental data was performed and in general, good agreement was found.

5 Conclusion

The contributions of DNS to turbulence research in the last decade have been impressive and the future seems bright. The greatest advantage of DNS is the stringent control it provides over the flow being studied. It is expected that as flow geometries become more complex, the numerical methods used in DNS will evolve. However, the significantly higher numerical fidelity required by DNS will have to be kept in mind. It is expected that use of non-conventional methodologies (e.g. multigrid) will lead to DNS solutions at an affordable cost, and that development of nonlinear methods of analysis are likely to prove very productive.

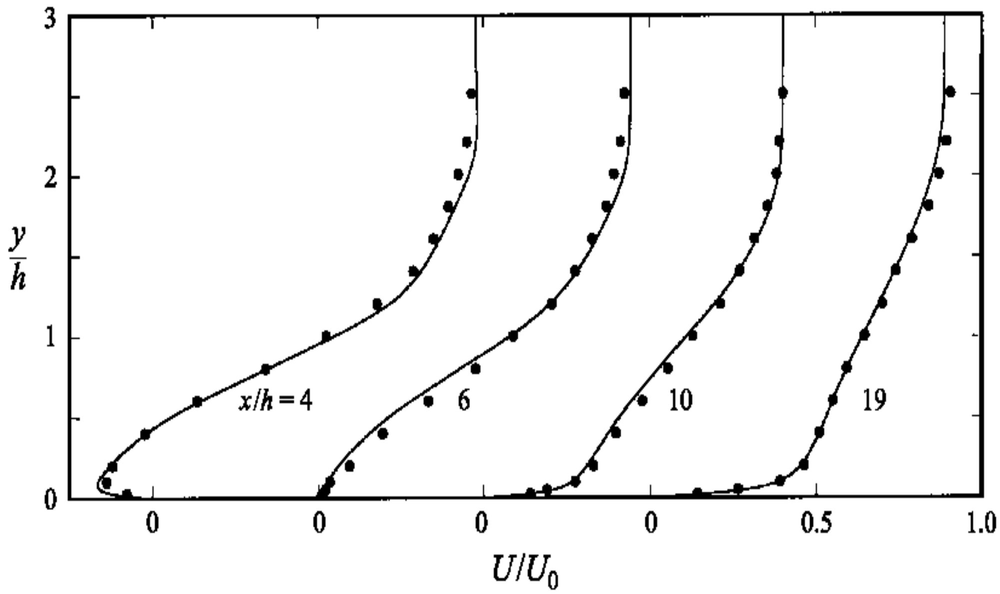

Figure 1: Comparison of mean streamwise velocity profiles generated by DNS of turbulent flow over a backward-facing step (Le *et al.* [7]) with experimental data obtained by Jovic & Driver [5]

The Reynolds number of the simpler turbulent flows are currently approaching those of the smaller-scale experiments. DNS of forced isotropic turbulence has been conducted on 512^3 grids by several workers with the help of parallel computers. The Reynolds number in these computations actually exceeds that in most laboratory experiments. DNS is most important in problems where simplification to the governing unsteady, nonlinear equations have not as yet been adequately validated.

Databases generated by DNS [13] provide results on turbulent flow statistics which are in good agreement with experiments thus greatly increasing the confidence in the technology.

These databases also offer the opportunity to extract information from the flow field which cannot, or only with much difficulty, be obtained from experiments. The availability of DNS data has resulted in novel approaches to model evaluation and allows testing of the concepts behind a model. DNS data is extensively used to evaluate LES results which are an order of magnitude faster to obtain. The availability of this detailed flow information has certainly improved our understanding of physical processes in turbulent flows which thus emphasizes the importance of DNS in present scientific research. Due to the very good correlation between the DNS results and the experimental data, DNS has become synonymous with the term “Numerical Experiment”.

References

[1] Haecheon Choi and Parviz Moin. Effects of the computational time step on numerical solutions of turbulent flow. *J. of Comp. Phys.*, 113:1–4, 1994.

[2] B.D. Duncan and K.N. Ghia. An iterative approach for solving the incompressible Navier-Stokes equations for simulation of transition and turbulence in complex geometries. *First International Conference on DNS and LES, Ruston, Lousiana* (see http://www.cfdrl.uc.edu/˜bduncan/afosr97/afosr97paper.pdf), August 1997.

[3] W.J. Feiereisen, W.C. Reynolds, and J.H. Ferziger. Numerical simulation of a compresssible, homogeneous turbulent shear flow. *Rep. TF-13, Thermosci. Div., Dept. Mech. Eng., Stanford*, 1981.

[4] Ronald D. Joslin. Discussion of DNS: Past, Present and Future. *First International Conference on DNS and LES, Ruston, Lousiana* (see http://techreports.larc.nasa.gov/ltrs/), August 1997.

[5] S. Jovic and D.M. Driver. Backward-facing step measurements at low Reynolds number, $Re_h = 5000$. *NASA Tech. Memo 108807*, 1994.

[6] John Kim, Parviz Moin, and Robert Moser. Turbulence statistics in fully developed channel flow at low reynolds number. *J. of Fluid Mech.*, 177:133–166, 1987.

[7] Hung Le, Parviz Moin, and John Kim. Direct numerical simulation of turbulent flow over a backward-facing step. *J. of Fluid Mech.* (see http://www.journals.cup.org/), 330:349–374, 1997.

[8] S.K. Lele. Compact finite-difference schemes with spectral-like resolution. *J. of Comp. Phys.*, 103:16–42, 1992.

[9] P. Moin and P.R. Spalart. Contribution of numerical simulation data to the physics, modeling, and measurement of turbulence. *NASA Tech. Memo 100022*, 1987.

[10] Parviz Moin and Krishnan Mahesh. Direct Numerical Simulation: A Tool in Turbulence Research. *Annual Review in Fluid Mech.*, 30:539–78, 1998.

[11] Yang Na and Parviz Moin. Direct numerical simulation of turbulent boundary layers with adverse pressure gradient and separation. *Rep. TF-68, Thermosci. Div., Dept. Mech. Eng., Stanford*, 1996.

[12] S.A. Orszag and G.S. Patterson. Numerical simulation of three-dimensional homogeneous isotropic turbulence. *Phys. Rev. Lett.*, 28:76–79, 1972.

[13] S. Parneix and P. Durbin. A new methodology for turbulence modelers using DNS database analysis. *CTR, Annual Research Briefs 1996, Stanford* (see http://www-fpc.stanford.edu/CTR/ResBriefs96/parneix.ps.Z), 1996.

[14] Man Mohan Rai and Parviz Moin. Direct simulations of turbulent flow using finite-difference schemes. *J. of Comp. Phys.*, 96:15–33, 1991.

[15] R.S. Rogallo. Numerical experiments in homogeneous turbulence. *NASA TM 81315*, 1981.

[16] P.R. Spalart. Direct numerical simulation of a turbulent boundary layer up to $R_\theta = 1410$. *J. Fluid Mech.*, 187:61–98, 1988.

[17] D.C. Wilcox. Turbulence modeling for CFD. *DCW Industries, La Canada, California*, 1993.