DISCUSSION OF DNS: PAST, PRESENT, AND FUTURE

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Abstract

This paper covers the review, status, and projected future of direct numerical simulation (DNS) methodology relative to the state-of-the-art in computer technology, numerical methods, and the trends in fundamental research programs.

1. INTRODUCTION

Most review articles tend to present an exhaustive list of research publications documenting the status of a technology. Review papers by Kleiser and Zang[1] and Reed[2] list such a treasure of literature on direct numerical simulation (DNS) applied to boundary-layer transition. In addition, discussions relating to issues for compressible DNS[3-6] and the use of DNS for turbulent flows[7,8] are available to the interested reader. In this short essay, it would be more valuable to look at DNS in the light of required technologies than to rehash or condense the available literature within the present page limitations. Hence, this paper will take a different twist on DNS of the past and look at future computations subjective to the author's views.

2. COMPUTATIONAL FLUID DYNAMICS

Computational Fluid Dynamics, usually abbreviated as CFD, has been used to refer to the computational solution of fluid dynamics problems. In 1976, Chapman[9] showed a progression of CFD capability with time (Table 1). Using computer-speed forecasts, viscous time-averaged and time-dependent CFD were projected to be possible during the late-1970s and mid-1980s. Here, we are in the late-1990s and both the viscous time-averaged solutions are possible but some controversy surrounds accuracy and interpretation of the results. Time-dependent solutions are now possible on simplified geometries and at low Reynolds numbers. Also because CFD is an all-encompassing term (or "buzz-word") which has been used to cover fluid mechanics from linear ordinary differential equations through full unsteady nonlinear Navier-Stokes equations, a hint of skepticism naturally arises when discussing the value of CFD results. This skepticism (at times) has led to the humorous *Color Fluid Dynamics* and has implied some mystical skills are required to obtain CFD results. In some sense, significant experience is required to interpret the CFD obtained solutions, lending to the assumptions/limitations of any given code. To help clarify the adequacy of a solution, perhaps every future paper or presentation which makes use of CFD (or a code name, such as CFL3D, TLNS3D, etc) should not only state that the Navier-Stokes equations are not solved directly but rather they are modeled and highlight the limitations of the results due to the assumptions within the methodology (e.g., low-order methodologies utilized, potential turbulence model limitations, inadequate grid resolution, etc.). Hence, we should change the paradigm of our engineers and managers from CFD implying a definitive (or exact) quantitative solution of the fluid and aerodynamic problem toward CFD as a tool which models the aerodynamics, which is ever striving for quantitative accuracy.

3. DIRECT NUMERICAL SIMULATION

Direct Numerical Simulation or Direct Navier Stokes (DNS) is a CFD technology implying a nearly exact solution to a unsteady, nonlinear governing systems of equations. 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. Table 2 shows the progression of DNS usage through 1997. A computer search of the literature indicates that an exponential growth in the use of DNS as a CFD methodology has occurred. Like conventional CFD, a state of overuse of terminology may be appearing in the literature. Although the scientific community can gleam the limitations inherent in the use of DNS in a given study, decision making managers or those reviewing manuscripts may not be familiar with such limitations. Furthermore, because DNS has become equivalent to "exact solution," discrepancies in solutions, or comparisons, may be incorrectly attributed to behavior of the aerodynamics (flow physics) or to faults in experiments or theory.

Table 1. Status of computational aerodynamics.[9]

Stage of approximation	Readiness time period 2D 3D 3D Airfoils Wings Aircraft	Limitations	Pacing Item
Inviscid linearized	1930's 1950's 1970's Used in current aircraft design	Slender configurations Small angle of attack Perfect gas No transonic flow No hypersonic flow No flow seperation	
Inviscid nonlinear	1971 1973 1976 ? Development nearing completion	No flow seperation	Code development
Viscous time averaged	1975 1977 ? 1979 ? Early stage of development	Accuracy of turbulence model	Turbulence modeling
Viscous time dependent	Mid 1980's	Accuracy of Navier - Stokes equations	Development of advanced computer

Table 2. Use of Direct Numerical Simulation (DNS) in the literature.

Year	Citations
before 1970	0
1970-79	12
1980-89	116
1990-97	536

Perhaps the CFD and DNS community have suffered because the terminology has lacked sufficient definition to discriminate between the various levels of approximation of the governing equations. In some cases, DNS has been used for studies where the temporal and spatial resolutions have been insufficient to capture the quantitative behavior of the fluid dynamics. Hence, the sub-grid scale structures have been modeled in an ad hoc manner. Unresolved solutions often have value to study qualitative features of the problem in a less costly manner compared to a fully resolved study. Perhaps, we need to agree on what DNS implies and when DNS becomes an ad hoc LES procedure, and what we term conventional CFD. Perhaps additional definitions or conventions for the use of these terms and the introduction of some new abbreviations are in order. Some of these may take the form Course-Grid DNS (CGDNS) or ad-hoc LES (AHLES) or steady, low-order CFD (SLOCFD).

Returning to the subject matter—past, present and future of DNS, the technical challenges associated with DNS involve extreme memory and computational speed re-

quirements. Concerning memory, 3D simulations of solar convection, for example, could require on the order of 10^{30} grid points.[10] Simulations of a planetary boundary layer could require 10^{18} grid points,[10] while computers of the 1990s can handle only about 10^9 grid points. Concerning performance, DNS could be attainable for flow past an airfoil ($Re \simeq 10^8$) if teraflop (10^{12} flops) performance wave available. With exaflop (10^{18} flops) performance, DNS could be enabled for flow past a complete aircraft[11]. Extending the use of DNS to more complex configurations is significantly linked to computer advancements and/or novel faster, and more accurate algorithms. And clearly, because LES is a fraction of the cost of DNS, large-eddy simulations have the potential to make large contributions to the aerospace industry before full scale DNS is possible. Hence, my remaining comments apply to LES as well as DNS.

4. COMPUTER ADVANCES

From the 1976 presentation by Chapman,[9] computer speed versus year the computer was available is reproduced in our figure 1 and amended to include additional Cray products and a projected computer with pentaflop performance in 2010. In relation to the predicted performance gains of 81%/year and 112%/year, computer technology advances have slowed.
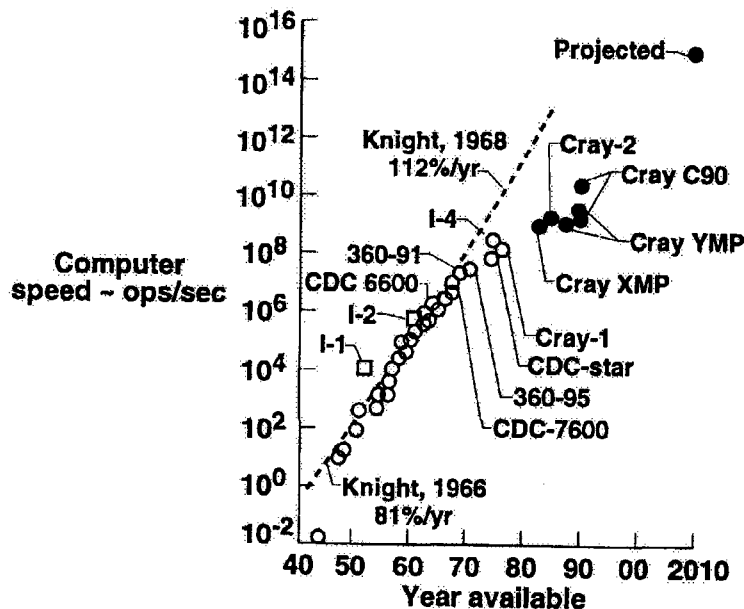

Figure 1. Computer speed versus year available.[9]

In addition to raw computer speed advances, numerous multi-processor, parallel computers have entered the market for potential use in solving engineering and science problems. Intel IPSC/860 and Paragon, IBM SP1 and SP2, and various other computers have been used to examine the feasibility of CFD on parallel architectures. Shown in figure 2 are the cost of major kernels of a spatial DNS code,[12] the communication cost, and the total computing cost on the IBM SP2. Clearly, the SP2 becomes competitive with the same code using one processor of a Cray C90, in spite of the communication penalty incurred with a parallel computer.

Also shown in figure 2, a single 3D computational domain can be conveniently (and efficiently) split among the processors by dividing the domain equally among the computing nodes (division among 4 nodes is shown for example in figure 2). So parallel computers

potentially buy performance gains and additional memory for the application of DNS to larger problems. For example, using a parallel computer, teraflop (10^{12} flops) performance could be attainable and should enable DNS of flow past an airfoil.
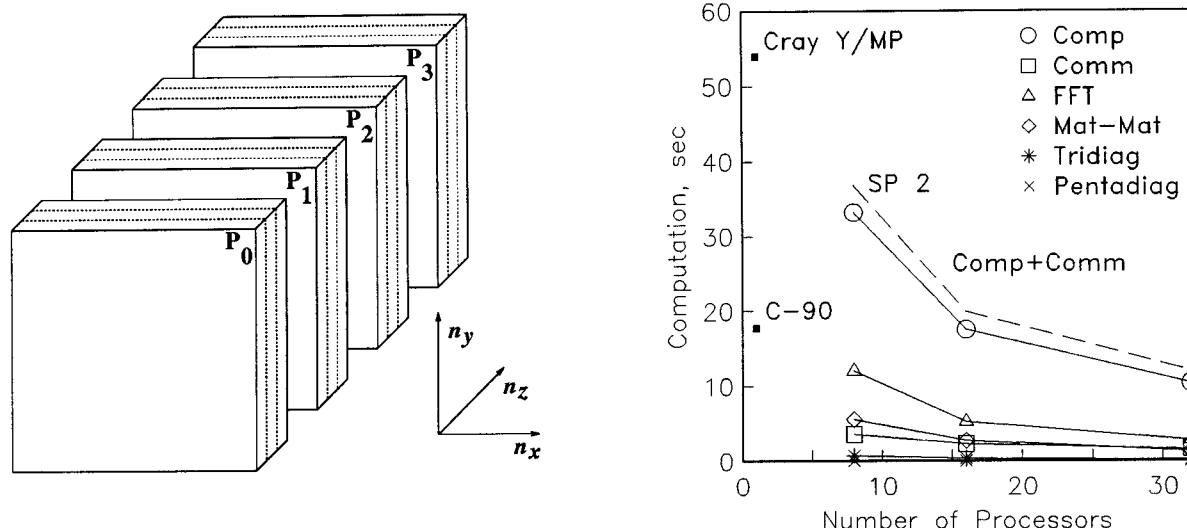

Figure 2. Domain decomposition for parallel computing and computer cost versus number of processors.[12]

5. NUMERICAL/ALGORITHMIC METHODS

While the speed increases bought by faster computers goes significantly to what can be accomplished using DNS, smarter programming, faster algorithms, and novel theoretical tools should 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,[13] high-order compact difference techniques have been included in more recent DNS efforts. Spectral-element methods have been used for spatial discretization around complex geometries.[14,15] Chebyshev collocation techniques have been used in boundary-layer and channel flow problems,[16] and a fully 3D non-periodic code has used used Chebyshev collocation techniques in two coordinate directions and compact and finite differences in the third coordinate direction.[17] Numerous DNS studies have used Adams-Bashforth, Runge-Kutta, Crank-Nicolson, and time-splitting approaches for time advancement.

In the future, more advanced approaches should be considered. For example, a multigrid general geometry DNS approach[18-21] has been developed and tested on a workstation. This multigrid DNS (MGDNS) approach has enabled computations of transition induced by 2D and 3D roughness and 3D transition on an unswept airfoil.

Benefits obtained through careful programming and by updating the algorithms of a DNS code can be demonstrated by the example in Table 3. Using a Cray YMP supercomputer, a DNS code was updated over a five-year period. Using the same grid and test problem, Table 3 clearly shows that both memory reductions and speed enhancements can be realized with minimal effort. (Note, the increase in cost per time step is attributed to a more expensive time-step procedure which buys a significantly lower number of time steps per period of computation.)

Table 3. Program and Algorithmic developments for use in DNS.

	1990	1995
Memory (Mb)	87.6	35.7
Startup Cost (sec)	1896	51
Cost/Time step (sec)	20.3	48.37
Cost/Period (hr)	17	4

Often Poisson or Helmholtz equations must be solved during the course of a DNS. A Gauss-Seidel-like line iteration procedure[22] and direct solvers[17,23] have been used in DNS codes for Poisson/Helmholtz equations. With engineering and scientific applications as the customer, fast serial and parallel high-order direct solvers for Poisson[24] and Helmholtz[25] equations (Dirichlet and Newmann boundary conditions) have been tested for speed and accuracy.

Using computer-specific libraries and attributes can buy DNS significant improvements in compute power. For example, the CRAY BUFFER IN/OUT allows asynchronous read/writes to disk. When the command is executed, data on a disk can be accessed simultaneously while the code "crunches" numbers. On parallel computers, asynchronous communication enables computations to proceed while information is exchanged among the nodes.

6. BOUNDARY CONDITIONS

Boundary conditions have always been a critical issue in the use of DNS. Kloker et al.[22] summarized most of the available outflow treatments: outflow moving boundaries[26] and the imposition of a non-physical region at the end of the physical region. In this non-physical region (or zone), a favorable pressure gradient or suction,[26] increased viscosity,[19,21] the Fringe method,[27] and the buffer domain technique[28] have been demonstrated to minimize non-physical reflections at the outflow.

Pruett et al.[5] noted the boundary condition difficulties with high speed applications due to artificial Mach waves (and reflections) if the disturbance forcing, far-field boundary conditions and downstream conditions are not carefully handled.

In the far-field, the 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.[29]

7 FUNDAMENTAL FLUID MECHANICS

There are many issues related to fundamentals in fluid mechanics where DNS (and LES) can play an important role. For example, we know that the flow along the attachment-line of swept wings is laminar or turbulent depending on the Reynolds number. The experimental and theoretical results agree for the linear critical Reynolds number where small-amplitude disturbances become unstable on the attachment line at $R_\theta \simeq 245$.[30-34] For large-amplitude disturbances, turbulence decays below some critical Reynolds number and transition to turbulence will occur above this point. At this critical point, transition bypasses the conventional linear instability breakdown process. The experiments[35-38] showed that disturbances are damped for $R_\theta < 100$ and the flow becomes turbulent for $R_\theta > 100$. Note, the wide gap between the linear critical Reynolds number of $R_\theta \simeq 245$ and the turbulent suppression critical Reynolds number of $R_\theta \simeq 100$. Bridging this gap is important for wing design. Because of the wide spectrum of potential disturbances in the flow, DNS is required to resolve this gap.

Concerning the fluid mechanics phenomena of local/global and absolute/convective instability,[39] DNS can play an important role in validating new theoretical concepts where traditional temporal or spatial theoretical approaches are alone invalid. For example, simulations which excite (forced actuation) global instabilities (in regions where the global instabilities may be marginally stable) can aid enhanced mixing.

The unsteady flow about complex configurations have been studied[14,15] using DNS and should continue toward understanding physics and to devise/validate simplified design tools. For example, impulsive flows[14] (transient phenomena) have been computed about a complex wedge configuration.

7.1 ACTIVE FLOW CONTROL

In the last decade, increased attention has been devoted to the development of mechanical, distributed, and micro-sized techniques capable of enhancing our ability to measure and control the unsteady flow in a wide variety of configurations (e.g., engine inlets and nozzles, combustors, automobiles, aircraft, and marine vehicles). Controlling the flow in these configurations may lead to greatly improved efficiency and performance, while decreasing the noise levels generally associated with the otherwise unattended unsteady flow. Depending on the desired result, one might wish to delay or accelerate transition, reduce drag or enhance mixing. Furthermore, high-performance aircraft maneuvers without conventional mechanical devices may be a future goal (DOD, NASA, and industry funded programs). Removing conventional controls would lead to significant weight reductions.
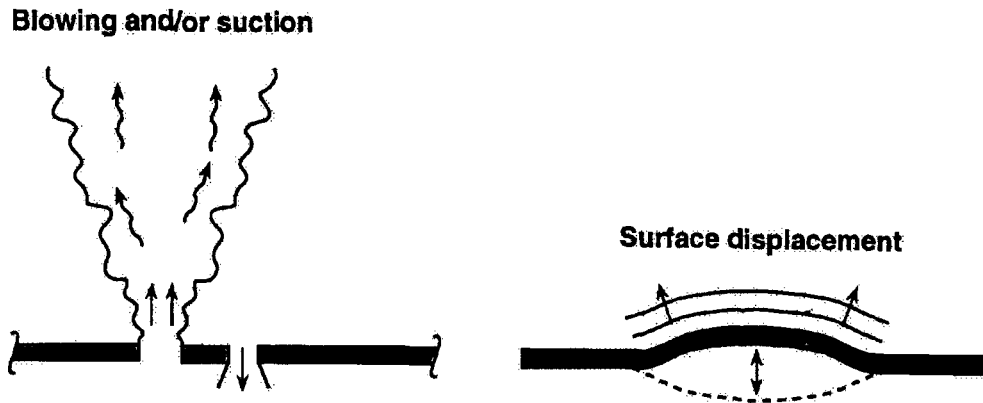
Blowing and/or suction

Surface displacement

Figure 3. Sketch of fluidic and surface displacement actuators.

7.1. Unsteady Actuator-Induced Flow Control

Aerodynamic design has a whole new set of challenges with the introduction of unsteady flow control. In particular, DNS (and LES) are required to identify the flow physics governing the coupled actuator-induced and shear flows (laminar through turbulent flow). The unsteady fluidic and surface displacement actuators (see figure 3) may involve zero, positive, or negative net mass, range in size from MEMS (less than 1 centimeter) to macro devices (centimeters), and operate at frequencies from 0 Hz to mili-Hz to kHz. Such active flow control concepts have been experimentally tested on an airfoil in a wind-tunnel.[40,41] The results suggest that enhanced lift over the angle-of-attack range is available through the use of unsteady fluidic actuators.

DNS can certainly be used to guide such experiments and to explain the complex fluid dynamics of the actuated flow field. To demonstrate the value of DNS, unsteady

incompressible Navier-Stokes simulations were accomplished for the flow field induced by a single zero-net-mass actuator.[42] The actuator had a distribution of

$$u(t,y)|_{x=0} = U_m \sin(\omega t) \cdot \sin(y/d) \tag{1}$$

where U_m is the maximum actuator velocity, ω is the forcing frequency, and d is the actuator orifice size. Here, the forcing distribution is simply half of a sine-wave period in the y-direction; however, the simulations can be repeated when experimental data suggests an an alternate distribution. For this example problem, $U_m = 20 m/s$, $\omega = 0.5$ ($\simeq$ 3183 Hz), and $d = 0.5$ mm are selected since these parameters are close to the family of synthetic-jet actuators.[43]

The computational domain had 201 grid points covering 18 mm in the jet-flow direction and 81 collocation points covering 16 mm in the cross-jet direction. The buffer domain begins 13.5 mm away from the actuator. Figure 4 shows contours of the u and v velocity components after 12 periods of forcing. Consistent with the experiments,[43] a jet-like flow develops in the simulations in spite of the zero net mass entering the computational domain. After reaching a peak amplitude close to the orifice, the amplitude of the jet begins to decay. Interesting to this fluidic actuator, a fairly strong transient phenomena is observed (in the middle of the computational domain) during the start-up of the actuation.
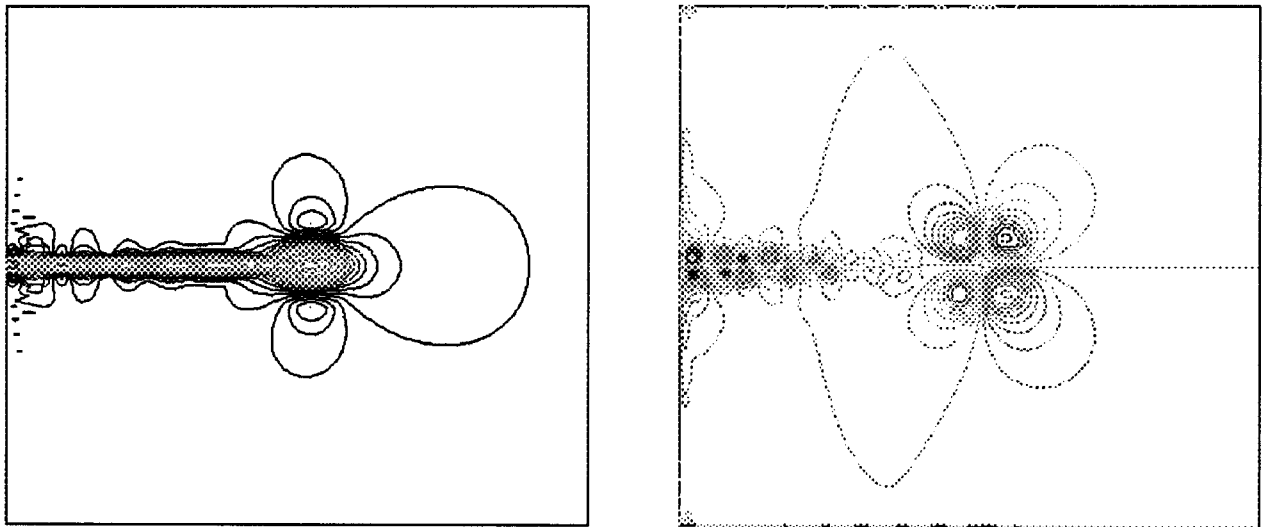

Figure 4. Contours of u- and v-velocities induced by zero-net-mass fluidic actuator.[42]

7.2 Control Theory

The coupling of control theory with DNS (or other unsteady nonlinear CFD approach) is necessary to expand our understanding of what kind of actuation is required for a given objective function. Being that actuation must be positioned on a surface of the configuration, the computations with control would be activated with a boundary condition. Such a concept would take the following form over a desired time interval $t \in (T_0, T_1)$, where $0 \leq T_0 < T_1 \leq T$.

$$u_i\Big|_{\Gamma_a} = \begin{cases} g_i & \text{in } (T_0, T_1) \\ 0 & \text{in } (0, T_0) \text{ and } (T_1, T) \end{cases} \tag{2}$$

Here, the control function $g_i(t, x)$ gives the rate at which fluid is injected, sucked, or the surface is displacement through the actuator Γ_a (prescribed dimensions of the actuator).

The actuator response based on the flow and objective function must be understood as a product of the optimization process.

For example, a self-contained methodology for active flow control[44,45] was developed using control theory and DNS. The method coupled the time-dependent Navier-Stokes system with the adjoint Navier-Stokes system and optimality conditions from which optimal states (i.e., unsteady flow fields and controls) were determined. The problem of transition delay was used as the initial validation case to test the methodology. The objective of control was to match the wall-normal stress to the steady base flow at a prescribed sensor location on the wall. Unlike feedback control methodologies wherein the sensed data determines the control through a specified feedback law or controller; the time-dependence of the control was the natural result of the minimization of the objective functional. Penalty terms were added to the functional to limit the size of the control g_i and the oscillations in time. Constants (for example, α_i and β_i) were used to adjust the relative importance of the terms appearing in the functional. A sensor was used to feed information to a controller that in turn fed information to the actuator. (In the optimal control setting, the sensor is actually an objective functional and the controller is a coupled system of partial differential equations that determine the control that does the best job of minimizing the objective functional.) Control was effected through the injection and suction of fluid through a single orifice on the boundary.

The method of Lagrange multipliers was formally used to enforce the constraints. Each argument of the Lagrangian functional was considered to be an independent variable so that each may be varied independently. For the incompressible Navier-Stokes equations, $\hat{u}_i$ were Lagrange multipliers that were used to enforce the x_i-components of the momentum equations, $\hat{p}$ was a Lagrange multiplier that was used to enforce the continuity equation, and s_i are Lagrange multipliers that were used to enforce the individual components of the boundary conditions (eqn. 2). The first variations of the Lagrangian with respect to the state variables u, v, and p were set equal to zero, leading to the *adjoint* or *co-state equations*.

$$-\frac{\partial \hat{u}_i}{\partial t} + \hat{u}_j \frac{\partial u_j}{\partial x_i} - u_j \frac{\partial \hat{u}_i}{\partial x_j} - \frac{\partial \hat{p}}{\partial x_i} - \nu \frac{\partial^2 \hat{u}_i}{\partial x_j \partial x_j}; \quad \frac{\partial \hat{u}_i}{\partial x_i} = 0 \qquad (3)$$

where the equations hold for $t \in (0, T)$.

$$\hat{u}_i \big|_{t=T} \qquad (4)$$

were initial conditions and homogeneous conditions were used everywhere on the computational boundary except where the sensor responds to the adjoint system. In the sample problem, the following forcing condition was used for the adjoint system.

$$\hat{u}_i = \alpha_i (\tau_i - \overline{\tau}_i) \quad \text{on} \quad (T_a, T_b) \times \Gamma_s, \qquad (5)$$

$\overline{\tau}_i(t, x)$ is a given function (desired result) defined on $(T_a, T_b) \times \Gamma_s$, where (T_a, T_b) is a time interval such that $0 \leq T_a < T_b \leq T$.

The *optimality conditions* were determined in a manner similar to the adjoint equation and are described by the equations below.

$$-\frac{\partial^2 g_i}{\partial t^2} + g_i = -\frac{1}{\beta_i} \left(\hat{\tau}_i \right) \quad \text{on} \quad (T_0, T_1) \times \Gamma_a \qquad (6)$$

and $g_i(t, x)$ is subject to initial and boundary conditions

$$g_i \big|_{t=T_0} = g_{i,0}(x) \quad \text{and} \quad \frac{\partial g_i}{\partial t} \bigg|_{t=T_1} = 0 \quad \text{on} \quad \Gamma_a \qquad (7)$$

Given $\hat{\tau}$ at each point $x \in \Gamma_a$, a two-point boundary value problem in time over the interval (T_0, T_1).

The coupled system was solved in an iterative manner. First, the simulation started with no control $(g_i = 0)$ and the Navier-Stokes equations were solved for the velocity (u, v) and pressure (p) fields. The adjoint equations were then solved for the co-state variables $(\hat{u}, \hat{v})$ and $\hat{p}$. Then, using these adjoint variables, the optimality conditions were solved. The procedure was repeated until satisfactory convergence is achieved.

Here, the optimal control methodology was applied to a boundary-layer flow having a single instability wave that can be characterized by a discrete frequency within the spectrum. These discrete small-amplitude instabilities can be suppressed through *wave cancellation* (WC), or wave superposition, using known exact information concerning the wave. Hence, the optimal control is "known" and can be used to validate the present DNS/optimal control theory approach in which the instability is to be suppressed without any a priori knowledge of said instability. For the computations, the grid has 401 streamwise and 41 wall-normal points. The free-stream boundary is located $75\delta_o^*$ from the wall, and the streamwise length is $224\delta_o^*$ which is equal to approximately 8 Tollmien-Schlichting (TS) wavelengths. The nondimensional frequency for the forced disturbance is $F = \omega/R \times 10^6 = 86$; the forcing amplitude is $v_f = 0.1\%$. The Reynolds number based on the inflow displacement thickness (δ_o^*) is $R = 900$. To complete one iteration of the active-control simulation process, 4.5 min. on a Cray C-90 are required using a single processor for a iteration defined as three periods $(T_a \to T_b = 3T_p)$ of disturbance forcing.

Based on $\alpha_2 = 1$ (selected arbitrarily) and $\beta_2 = 16.5$ (refined through feedback method), the converged solution was obtained in 4 iterations. The wall-normal velocity (v) at a fixed distance from the wall and the actuator response (g_2) is shown in figure 5 and compared with the desired wave-cancellation (WC) solution and a amplified uncontrolled solution. These results yield a delay in the transition by-way-of a suppression of the instability evolution.
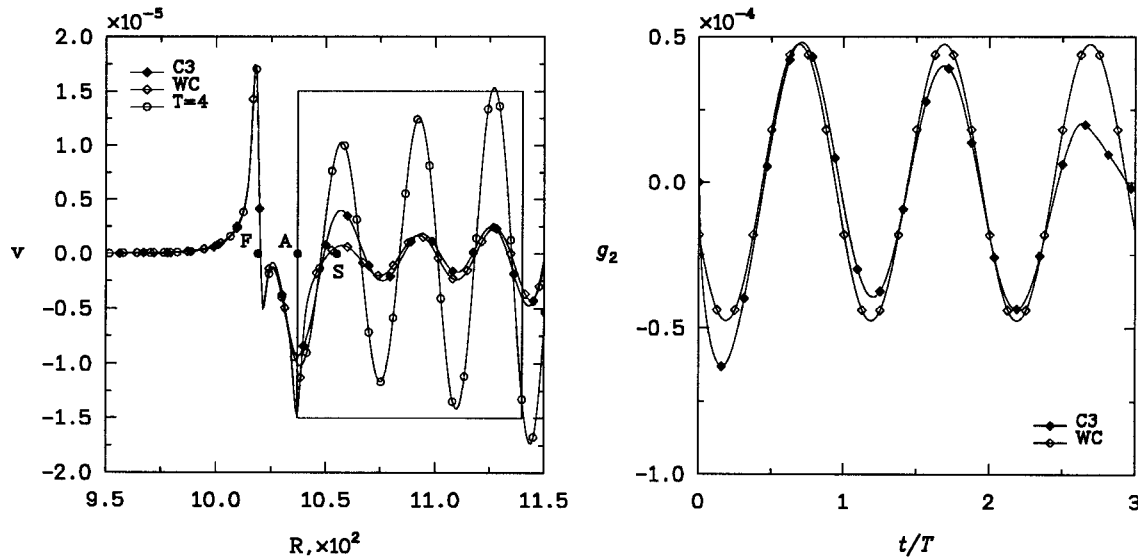

Figure 5. Disturbance wall-normal velocity and actuator response with downstream distance for control (C3) and wave cancellation (WC).[44] (F-forcing location, A-actuator location, and S-sensor location).

The ultimate goal of this line of research is to introduce automated control to external flows over realistic configurations such as wings and fuselages, and to guide the development of actuators and control laws. The methodology may potentially be applied to separation control, re-laminarization, and turbulence control applications using one or more sensors and actuators. As DNS becomes useful in larger, more complex problems (by-way-of computer speed advancements, parallel computing, advanced algorithm development), such controller approaches can guide active flow control projects.

Finally, reducing the memory requirements of such methodologies is a primary task for future research. The adjoint system (eqn. 3) requires that the velocity field (u, v) obtained from the Navier-Stokes equations be known in the computational domain for all time. For this sample 2D problem, the iteration sequence and a modestly course grid, 246 Mb of disk (or runtime) space are required to store the velocities at all time steps and for all grid points. Clearly for 3D problems the memory requirements becomes prohibitively expensive. This limitation can easily be removed if the flow-control problem involves small-amplitude unsteadiness (or instabilities). The time-dependent coefficients of the adjoint system reduce to the steady-state solution and no addition memory is required over the Navier-Stokes system. Perhaps, the coefficients may be stored every 10 (or more) time-steps or may be represented by a statistical average of the flow, thereby reducing the memory requirements by an order of magnitude. This hypothesis will require validation in a future study.

CONCLUSIONS

Based on the author's subjective view, DNS will have limited growth on one-processor computers; however, parallel computers will enable solutions to a larger class of problems. Nonconventional methodologies (e.g., multi-grid) will lead to DNS solutions at an affordable cost. DNS must be used in problems where simplification to the governing unsteady, nonlinear equations have not as yet been adequately validated. In the 1990s and beyond, such flows include active flow control on simple and complex configurations and traditional transition and turbulent shear flows on complex configurations.

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