Luigi Martinelli
Associate Professor
Department of Mechanical and
Aerospace Engineering,
Princeton University,
Princeton, NJ 08544
e-mail: martinel@princeton.edu

Antony Jameson
Thomas V. Jones Professor of Engineering
Department of Aeronautics and Astronautics,
Stanford University,
Stanford, CA 94305
e-mail: jameson@baboon.stanford.edu

Computational Aerodynamics: Solvers and Shape Optimization

Aeronautics, and in particular aerodynamics, has been one of the main technological drivers for the development of computational fluid dynamics (CFD). This paper presents a personal account of the main advances in the development of solvers and shape optimization techniques, which have contributed to make CFD an essential part of the design process of modern aircraft. [DOI: 10.1115/1.4007649]

Keywords: computational fluid dynamics, aerodynamics, shape optimization

1 Introduction

Since the development of the IAS computer built from 1942 to 1951 at the Institute of Advanced Studies under the supervision of John von Neumann, computer engineers' push to make the hardware more practical and efficient has been driven and challenged by a handful of applied fields. While it is widely recognized that Aerodynamics played a key role in the development of modern scientific computing, it is instructive to understand why. We argue that the trigon formed by a compelling technological problem, the availability of useful mathematical models of increasing complexity, and the relentless pace of improvement in computing platforms imposed by Moore's law, is responsible for the amazing advances in computational aerodynamics of the past 50 yr. Moreover, the particular nature of the aerospace industry imposes on computational aerodynamics stringent requirements on both the accuracy and robustness of the computations, which provided the need and the impetus for the development of advanced numerical techniques. This set of circumstances has brought and maintains computational aerodynamics at the forefront of modern scientific computing.

In the early dawn of aviation, empiricism dominated aerodynamic design. Airfoil shapes were selected based on observation of nature (e.g., lilienthal) or good physical insight and new designs evolved following a build-test-modify process. By the late 1930 s, a deeper theoretical understanding of airfoil performance at subsonic speeds had been gained primarily thanks to Prandtl's and Glauert's pioneering work. This approach culminated in the development of the NACA 6 series of airfoils, which was obtained by hand calculations using the Theodorsen method for conformal mapping. Nevertheless, wind tunnel testing remained the main tool for aerodynamic analysis and design. The quest for supersonic flight, initiated in the late 1930's in Germany and Italy, had moved after World War II to the USA and the USSR, and the onset of the cold war exacerbated the technological competition between the two superpowers. The Mig 19, the first mass-produced true supersonic fighter (Mach 1.35), entered production in 1955, and was faster than the F-100 Super Saber, which was only capable of Mach 1.05 in level flight. By the end of the decade the speed had topped Mach 2.00 with the F104 (1958) and the Mig21 (1959). Again, advances were made principally by superior physical insight confirmed by wind tunnel tests. The discovery of the area-rule by Richard T. Whitcomb, his development of supercritical airfoils, and later of winglets are among the most notable examples of this traditional build-test-modify approach. This process was expensive, and in the 1960 s cost escalated with the complexity of newer projects. For example, more that 20,000 h of wind tunnel testing were needed for the development of the F111 or the Boeing 747. The need of gaining air-superiority together with the explosive growth of civil air traffic consolidated the strategic importance of aeronautical sciences in general and aerodynamics in particular.

By 1960, it began to be apparent that digital computers had improved to the point of making it possible to attempt their use for the calculation of the aerodynamic characteristics—at least of isolated aircraft components—by solving a suitable mathematical model. The conservation of mass, momentum and energy for a viscous Newtonian fluid, which are generally referred to as the Navier–Stokes equation, govern the dynamics of any flow under the assumption that the fluid is a continuum; they have been known for approximately 150 yr, but solution of this nonlinear set of partial-differential equations is still daunting. Fortunately, since efficient flight can be achieved only by establishing highly coherent flows, useful predictions can be made with simplified mathematical models. In particular, since the Reynolds' number of a typical aircraft is of the order of 10^7, aerodynamic forces such as lift, Induced drag and in the case of transonic or supersonic flight wave-drag, can be computed by using inviscid flow models. It was precisely the availability of a hierarchy of models of increased complexity and fidelity, which yield useful prediction at different stage of a design, that allowed computational aerodynamics to develop in-step with Moore's law. The 1960s were dominated by the development of boundary integral methods (panel methods) based on the solution of a linear-potential equation both for purely subsonic or supersonic flow, for arbitrarily complex geometry [1–3].[1]

The late 1960s and early 1970s have witnessed the emergence of computational fluid dynamics for more general industrial problems. In this wider arena, Spalding's group at Imperial College led the way. The split treatment of the pressure terms, which culminated in the development of the SIMPLE method [5], was born from unmatched physical insight as much as it was grounded in the mathematical properties of the equations. The development of advanced numerical methods coupled with the path-breaking advances in turbulence modeling made in the same period by Launder and Spalding [6] enabled the practical use of CFD in an industrial setting.

In aeronautics, prediction at transonic speeds were needed. The importance of the transonic flight regimes is twofold. To a first approximation, cruising efficiency is proportional to ML/*D*, the product of the Mach number *M* with the lift *L* to drag *D* ratio (aerodynamic efficiency). Since the aerodynamic efficiency is insensitive to the velocity, as long as shock waves are not present,

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[1]A more recent article by Hess [4] offers a comprehensive review of this approach.

it pays to increase the flight speed and cruise in the transonic regime. Moreover, military aircraft maneuver in transonic flow, and with the quest for high angle of attack maneuvering came the danger of abrupt wing stall (AWS). Thus, in the 1970s, the battleground shifted to the transonic regime, which requires the solution of a potential equation of mixed-type (elliptic/hyperbolic) either linearized or not. As a result, the first satisfactory methods for treating the nonlinear equations of transonic flow [7–12] and the hodograph method for the design of shock free supercritical airfoils [13] were developed.

In the 1980s, the attention shifted to the solution of the Euler equations and, later in the decade, to the Reynolds averaged Navier–Stokes (RANS) equations. The last twenty years have seen advances in the ability of predicting the flow on geometrically complex configurations, as well as renewed efforts toward the accurate simulation of time-dependent flow. Several accounts on the development of numerical methods for inviscid flow models—either based on a velocity potential equation or the Euler form of the conservation laws—have already appeared in the literature [14]. In this paper, we focus on methods suitable for the numerical solution of viscous models—either the Navier–Stokes equations or an averaged form of it augmented by a suitable turbulence model for closure, and present an account of our research on the subject, which spans more than two decades of development.

The ultimate goal of aerodynamics is not the analysis of the flow as much as it is the drawing of appropriate forms that enable the designer to meet the mission requirements with maximum efficiency and minimum cost. In the last two decades, the ultimate goal of developing a tool for automatic shape optimization using high-fidelity physical models has been realized. By casting the shape optimization problem as a control problem—the shape of the boundary being the control—constrained by a suitably chosen set of partial-differential equations (the flow model), adjoint-based design methods have been developed and gained acceptance in industry, becoming one of the main tools for aerodynamic design. The second part of this paper is an account of the development of adjoint-based shape optimization methods and their efficient implementation.

2 Solvers for Euler and RANS Equations

In a Cartesian coordinate system x_i, by assuming the standard Einstein summation convention on repeated indices, the conservation laws for a compressible fluid can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} = 0$$

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial \rho v_i v_k}{\partial x_k} + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{k_i}}{\partial x_k}$$

$$\frac{\partial \rho e_T}{\partial t} + \frac{\partial \rho h v_k}{\partial x_k} = \frac{\partial \tau_{k_i} v_i}{\partial x_k} + \frac{\partial}{\partial x_k} \kappa \frac{\partial T}{\partial x_k}$$

where

$$e_T = e(\rho, s) + \frac{\mathbf{v} \cdot \mathbf{v}}{2} = e(\rho, s) + \chi_E$$

and $h = (e_T + (p/\rho))$ is the enthalpy per unit mass. Also, for a Newtonian fluid

$$\tau_{i_k} = \lambda \frac{\partial v_l}{\partial x_l} \delta_{i_k} + \mu \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} \right)$$

if Stokes' postulate is applied $\lambda = -\frac{2}{3}\mu$. Also, heat conduction is modeled by the standard Fourier form, where κ is the coefficient of heat conduction. When the right hand side of these equations is neglected—for example, in the limit of high Reynolds' number—the equations reduces to the Euler form. It is well known that by Reynolds averaging—or mass-averaging—these equations one obtains a set of partial-differential equations for the mean flow that closely resembles the Navier–Stokes equations, but the averaging process gives rise to additional terms such as the Reynolds stress tensor that requires additional modeling. Hence, solvers developed for the Navier–Stokes equations are easily extended to the Reynolds averaged equations (RANS) provided that a suitable turbulence model is implemented for closure. (See paper by T. Gatski in this special edition.)

2.1 Discrete Formulation. The numerical solution of the conservation laws requires three steps:

(i) the discretization of the computational domain,
(ii) the representation of the PDEs on the discretized domain, both in space and time, and
(iii) the computation of the solution of the discretized equations.

If the computational domain is simply connected and bounded by uncomplicated shapes, this first step is almost trivial, but it becomes challenging even for a relatively simple two-element airfoil (i.e., a main foil plus a flap). The principal alternatives are Cartesian meshes, body-fitted curvilinear meshes, and unstructured, possibly tetrahedral, meshes. Each approach has *pros and cons* which have led to their use in particular applications. The Cartesian mesh minimizes the complexity of the algorithm at interior points and facilitates the use of high order discretization procedures, at the expense of greater complexity, and possibly a loss of accuracy, in the treatment of boundary conditions at smooth curved surfaces. This difficulty may be alleviated by using mesh refinement procedures near the surface. With their aid, schemes which use Cartesian meshes have been developed to treat very complex configurations [15–18].

Body-fitted meshes have been widely used, and are particularly well suited to the treatment of viscous flow since the grid spacing normal to a solid boundary can be clustered to provide adequate resolution of boundary layers. With this approach, the problem of mesh generation itself has proved to be a major pacing item. Procedures based on algebraic transformations [19–22], methods based on the solution of elliptic equations, pioneered by Thompson [23–26], and methods based on the solution of hyperbolic equations marching out from the body [27] form the core of the existing mesh generation software.

For very complicated configurations a multiblock approach is generally used in which the domain is first decomposed into several simpler subdomains (blocks). These blocks are then discretized using body-fitted curvilinear meshes. The domain decomposition can be such that there is a one-to-one matching of the faces of neighboring blocks. or there may be an overlap of the blocks yielding a so called overset mesh, as with the Chimera scheme [28,29].

Alternatively, the flow domain can be discretized by triangulation (tessellation). This yields a simplified domain discretization [30] process at the expenses of a more complex data structure, since in this case additional bookkeeping is required to identify neighboring cells. More recently, unstructured meshes have been extended to include arbitrarily shaped cells, such as prisms and pyramids [31]. A good review of CFD methods for unstructured meshes can be found in Ref. [32]. Alternative approaches such as meshless and immersed boundary methods, albeit promising, have not gained wide acceptance in aeronautics and will not be discussed further in this paper.

It is well known that a consistent representation of the PDEs on the discrete domain can be obtained either by developing approximate formulas for the operators directly, or by applying the exact operators to an approximation of the unknowns in a suitable basis. The first approach yields both finite difference and finite volume discretizations, while the latter represents a finite element approach.

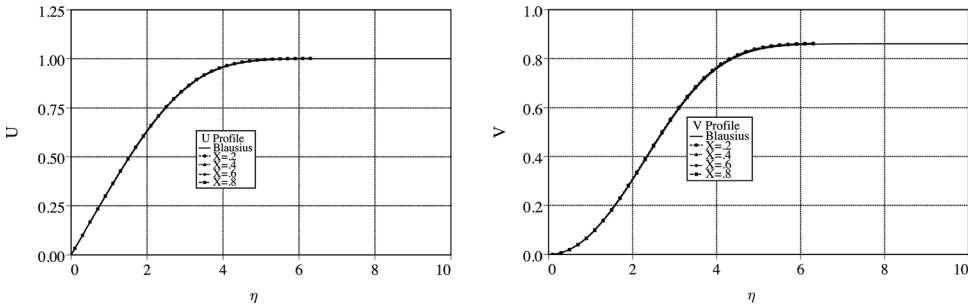

Fig. 1 Computed velocity profiles for 2D laminar boundary layer—finite volume cell-centered formulation with a CUSP dissipation. Similarity solution of both components of the velocity is verified.

The finite volume approach pioneered by Spalding and his collaborators at Imperial College in the late 1960s (as it is described in Ref. [33]), was introduced in computational aerodynamics by Paullay and MacCormack [34] in 1972, and to-date, it remains the most widely used discrete scheme.

An alternative route to the discrete equations is provided by the finite element method. Whereas the finite difference and finite volume methods approximate the differential and integral operators, the finite element method proceeds by inserting an approximate solution into the exact equations. The Dassault-INRIA group led the way in developing a finite element method for transonic potential flow. They obtained a solution for a complete aircraft (Falcon 50) as early as 1982 [35]. Euler methods for unstructured meshes have been the subject of intensive development by several groups since 1985 [36–40], and Navier–Stokes methods on unstructured meshes have also been demonstrated [41–43] as early as the early 1990s.

It is possible to verify that the finite difference and finite volume methods lead to essentially similar schemes on structured meshes, while the finite volume method is essentially equivalent to a finite element method with linear elements when a tetrahedral mesh is used. Provided that the flow equations are expressed in the conservation law form, all three methods lead to an exact cancellation of the fluxes through interior cell boundaries, so that the conservative property of the equations is preserved. The important role of this property in ensuring correct shock jump conditions was pointed out by Lax and Wendroff [44].

The discretization schemes described lead to nondissipative approximations to the convective terms. Dissipative terms may be needed for two reasons. The first is the possibility of undamped oscillatory modes. The second reason is the need for the clean capture of shock waves and contact discontinuities without undesirable oscillations. These symptoms are present also when solving the Navier–Stokes equations in regions, away from solid boundaries, in which the mesh resolution is inadequate or the viscous terms becomes negligibly small. Starting from the path-breaking work of Godunov [45], a variety of dissipative and upwind schemes designed to have good shock capturing properties have been developed in the 1980s and 1990s [43,46–61]. Today, a well established understanding of the requirements for building robust and accurate shock capturing schemes exists. In particular the construction of nonoscillatory schemes based on a local extremum diminishing (LED) or essentially local extremum diminishing (ELED) principle [62,63] has produced a very robust class of methods that has proved to be both accurate and efficient for the simulation of transonic and supersonic viscous flow in conjunction with both characteristic, and convective upwind split pressure (CUSP) flux-splitting [64]. Another approach which has proved very successful is Liou's AUSM [65].

2.1.1 Discretization of the Viscous Terms. The discretization of the viscous terms of the Navier–Stokes equations requires an approximation to the velocity derivatives $\partial v_i/\partial x_j$ in order to calculate the tensor τ_{i_j}. Then, the viscous terms may be computed and included in the flux balance.

In order to evaluate the derivatives one may apply the Gauss formula to a control volume V with the boundary S.

$$\int_V \frac{\partial v_i}{\partial x_j} dV = \int_S v_i n_j dS$$

where n_j is the outward normal. This formula can be applied to both tetrahedral and hexahedral cell yielding

$$\overline{\frac{\partial v_i}{\partial x_j}} = \frac{1}{\mathrm{V}} \sum_{\text{faces}} \bar{v}_i n_j S \tag{1}$$

where $\bar{v}_i$ is an estimate of the average of v_i over the face. If v varies linearly over a tetrahedral cell this is exact. Alternatively, assuming a local transformation to computational coordinates ξ_j, one may apply the chain rule and evaluate the transformation derivatives $\partial x_i/\partial \xi_j$ by using the same finite difference formulas as the velocity derivatives $\partial v_i/\partial \xi_j$ In this case, $\partial v/\partial \xi$ is exact if v is a linearly varying function. This formula can be carried out for either cell-centered or vertex-based schemes. The most efficient implementation of these formulas requires the introduction of dual meshes for the evaluation of the velocity derivatives and the flux balance.

A desirable property is that a linearly varying velocity distribution—as in a Couette flow—should produce a constant stress and hence a null viscous flux balance. This property is not necessarily satisfied in general by finite difference or finite volume schemes on curvilinear meshes. Nevertheless, an accurate resolution of a laminar boundary layer can be obtained with 16–32 grid points normal to the boundary, as illustrated in Fig. 1.

In the case of an unstructured mesh, the weak form leads to a natural discretization with linear elements, in which the piecewise linear approximation yields a constant stress in each cell. This method yields a representation which is globally correct when averaged over the cells, as is proved by energy estimates for elliptic problems [13], but it yields formulas that are not necessarily locally consistent with the differential equations, when a Taylor series expansion is substituted for the solution at the vertices of the local stencil.

Anisotropic grids are needed in order to resolve the thin boundary layers which appear in viscous flows at high Reynolds numbers. Otherwise, an excessively large number of grid cells may be required. The use of flat tetrahedra can have an adverse effect on both the accuracy of the solution and the rate of convergence to a steady state. This has motivated the use of hybrid prismatic-tetrahedral grids in which prismatic cells are used in the wall regions [66]. A review of many of the key issues in the design of flow solvers for unstructured meshes is given by Venkatakrishnan [67].

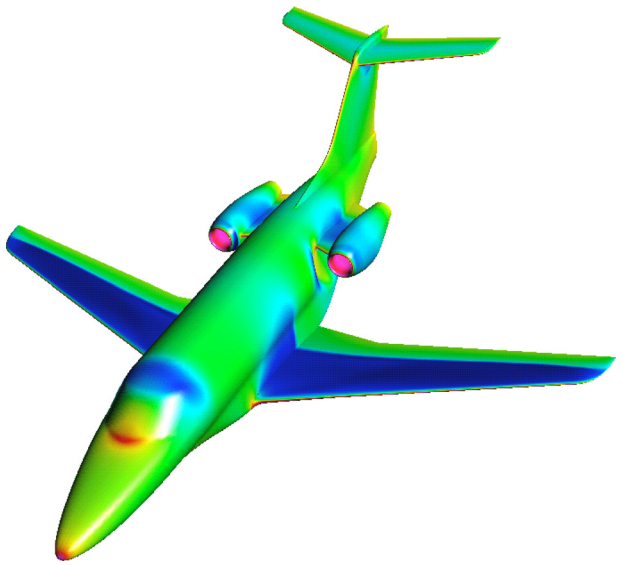

Fig. 2 Business jet configuration. Iso-C_P Navier–Stokes solution with 240 blocks and 5.8 million mesh points. $M = 0.82$, $\alpha = 1.0$ deg.

2.1.2 Time-Stepping Schemes. When the spatial operators are discretized separately from the time derivative, one obtain a set of coupled ordinary differential equations, which can be written in the form

$$\frac{\partial \mathbf{w}}{\partial t} + \mathcal{R}(\mathbf{w}) = 0 \tag{2}$$

where $\mathcal{R}(\mathbf{w})$ is generally called the residual symbol consisting of the flux balances defined by the space discretization scheme, together with the added dissipative terms. The name originates from the observation that, at a steady state, it must necessarily be $\mathcal{R}(\mathbf{w}) = 0$. If the objective is simply to reach the steady state and details of the transient solution are immaterial, the time-stepping scheme may be designed solely to maximize the rate of convergence. Both explicit schemes, in which the space derivatives are calculated from values of the flow variables at known at the beginning of the time step, and implicit schemes, in which the formulas for the space derivatives include unknown values of the flow variables, have been studied extensively. The permissible time step for an explicit scheme is limited by the Courant–Friedrichs–Lewy (CFL) condition, whereas implicit schemes are not. Thus, implicit schemes will require a smaller number of time steps to reach a steady state, which come at the expenses of an increase in the computational effort per time step. The prototypical implicit scheme can be formulated by estimating $\partial \mathbf{w}/\partial t$ as a linear combination of $\mathbf{R}(\mathbf{w^n})$ and $\mathbf{R}(\mathbf{w^{n+1}})$:

$$\mathbf{w}^{n+1} = \mathbf{w}^n - \Delta t\left\{(1-\mu)\mathcal{R}(\mathbf{w^n}) + \mu\mathcal{R}\left(\mathbf{w}^{n+1}\right)\right\}$$

This can be linearized as

$$\left(\mathbf{I} + \mu\Delta t\frac{\partial \mathcal{R}}{\partial \mathbf{w}}\right)\delta\mathbf{w} + \Delta t\mathcal{R}(\mathbf{w}^n) = 0$$

If one sets $\mu = 1$ and lets $\Delta t \to \infty$ this reduces to the Newton iteration, which has been successfully used in two-dimensional calculations [68,69]. In the three-dimensional case with, say, an $N \times N \times N$ mesh, the bandwidth of the matrix that must be inverted is of order N^2. Direct inversion requires a number of operations proportional to the number of unknowns multiplied by the square of the bandwidth of the order of N^7. This is prohibitive, and forces recourse to either an approximate factorization method or an iterative solution method.

Alternating direction methods, which introduce factors corresponding to each coordinate, are widely used for structured meshes [70,71]. They cannot be implemented on unstructured tetrahedral meshes that do not contain identifiable mesh directions, although other decompositions are possible [72,73]. If one chooses to adopt the iterative solution technique, the principal alternatives are variants of the Gauss–Seidel and Jacobi methods. A symmetric Gauss–Seidel method with one iteration per time step is essentially equivalent to an approximate lower–upper (LU) factorization of the implicit scheme [74–77]. On the other hand, the Jacobi method with a fixed number of iterations per time step reduces to a multistage explicit scheme, belonging to the general class of Runge–Kutta schemes [78]. Schemes of this type have proven very effective for wide variety of problems, and they have the advantage that they can be applied equally easily on both structured and unstructured meshes [79–82].

Radical improvements in the rate of convergence to a steady state can be realized by the multigrid time-stepping technique. The concept of acceleration by the introduction of multiple grids was first proposed by Fedorenko [83]. There is by now a fairly well-developed theory of multigrid methods for elliptic equations based on the concept that the updating scheme acts as a smoothing operator on each grid [84,85]. This theory does not hold for hyperbolic systems. Nevertheless, there is overwhelming evidence that multigrid methods accelerate the evolution of a hyperbolic system to a steady state [86–92]. Multigrid acceleration has proven extremely successful for the solution of the inviscid Euler equations, but less effective in calculations of turbulent viscous flows at high Reynolds numbers using the Reynolds averaged Navier–Stokes equations. The highly anisotropic grids required to resolve boundary layers and wakes, cause simple multigrid methods to yield fast initial convergence—albeit normally sufficient for engineering application—which generally slows down as the calculation proceeds to a low, less than optimal, asymptotic rate. This has motivated the introduction of semicoarsening and directional coarsening methods [93–99].

Multigrid methods have been applied on unstructured meshes by interpolating between a sequence of separately generated meshes with progressively increasing cell sizes [41,42,100,101]. It is not easy to generate very coarse meshes for complex configurations. An alternative approach, which removes this difficulty, is to automatically generate successively coarser meshes by agglomerating control volumes or by collapsing edges. This approach yields comparable rates of convergence and has proven to be quite robust [102–105].

Multigrid methods driven by optimized explicit time-stepping schemes, have been the preferred approach by the authors since they are naturally suitable for parallel computing. They were fully validated by the mid 1990s and they provide a quick and accurate prediction of viscous flow (Fig. 2).

Multigrid methods have also been applied to time-dependent calculations. In this case a multigrid explicit scheme can be used in an inner iterative loop to solve the equations of a fully implicit time-stepping scheme [106]. This method has proved effective for the calculation of unsteady flows that might be associated with wing flutter [107,108] and also in the calculation of unsteady incompressible flows [109]. It has the advantage that it can be added as an option to a computer program which uses an explicit multigrid scheme, allowing it to be used for the efficient calculation of both steady and unsteady flows. A similar approach has been successfully adopted for unsteady flow simulations on unstructured grids by Venkatakrishnan and Mavriplis [110].

3 Aerodynamic Shape Optimization

The use of computational simulation to scan many alternative designs has proved extremely valuable in practice, but it still suffers the limitation that it does not guarantee the identification of

the best possible design. Thus, the ultimate goal of computational simulation methods should not just be the analysis of prescribed shapes, but the automatic determination of the true optimum shape for the intended mission. This is the underlying motivation for the combination of computational fluid dynamics with numerical optimization methods.

Some of the earliest studies of such an approach were made by Hicks et al. [111,112]. The principal obstacle was the large computational cost of determining the sensitivity of the cost function to variations of the design parameters by repeated calculation of the flow. Another way to approach the problem is to formulate aerodynamic shape design within the framework of the mathematical theory for the control of systems governed by partial-differential equations [113]. In this view, the wing is regarded as a device to produce lift by controlling the flow, and its design is regarded as a problem in the optimal control of the flow equations by changing the shape of the boundary. If the boundary shape is regarded as arbitrary within some requirements of smoothness, then the full generality of shapes cannot be defined with a finite number of parameters, and one must use the concept of the Frechet derivative of the cost with respect to a function. Clearly such a derivative cannot be determined directly by separate variation of each design parameter, because there are now an infinite number of these.

Using techniques of control theory, however, the gradient of the cost function can be determined indirectly by solving an adjoint equation which has coefficients determined by the solution of the flow equations. The cost of solving the adjoint equation is comparable to the cost of solving the flow equations, with the consequence that the gradient with respect to an arbitrarily large number of parameters can be calculated with roughly the same computational cost as two flow solutions. Once the gradient has been calculated, a descent method can be used to determine a shape change which will make an improvement in the design. The gradient can then be recalculated, and the whole process can be repeated until the design converges to an optimum solution, usually within 50–100 cycles. The fast calculation of the gradients coupled with fast solvers makes optimization computationally feasible even for designs in three-dimensional viscous flow.

3.1 General Approach. For flow about an airfoil or wing, the aerodynamic properties which define the cost function are functions of the flow-field variables (w) and the physical location of the boundary, which may be represented by the function $\mathcal{F}$, say. Then

$$I = I(w, \mathcal{F})$$

and a change in $\mathcal{F}$ results in a change

$$\delta I = \left[\frac{\partial I^T}{\partial w}\right]_I \delta w + \left[\frac{\partial I^T}{\partial \mathcal{F}}\right]_{II} \delta \mathcal{F} \tag{3}$$

in the cost function. Here, the subscripts I and II are used to distinguish the contributions due to the variation δw in the flow solution from the change associated directly with the modification $\delta \mathcal{F}$ in the shape. This notation assists in grouping the numerous terms that arise during the derivation of the full Navier–Stokes adjoint operator, outlined later, so that the basic structure of the approach as it is sketched in the present section can easily be recognized.

Suppose that the governing equation R which expresses the dependence of w and $\mathcal{F}$ within the flow-field domain D can be written as

$$\mathcal{R}(w, \mathcal{F}) = 0 \tag{4}$$

Then, δw is determined from the equation

$$\delta \mathcal{R} = \left[\frac{\partial \mathcal{R}}{\partial w}\right]_I \delta w + \left[\frac{\partial \mathcal{R}}{\partial \mathcal{F}}\right]_{II} \delta \mathcal{F} = 0 \tag{5}$$

Since the variation $\delta \mathcal{R}$ is zero, it can be multiplied by a Lagrange Multiplier ψ and subtracted from the variation δI without changing the result. Thus, Eq. (3) can be replaced by

$$\begin{aligned}\delta I &= \frac{\partial I^T}{\partial w}\delta w + \frac{\partial I^T}{\partial \mathcal{F}}\delta \mathcal{F} - \psi^T\left(\left[\frac{\partial R}{\partial w}\right]\delta w + \left[\frac{\partial R}{\partial \mathcal{F}}\right]\delta \mathcal{F}\right) \\ &= \left\{\frac{\partial I^T}{\partial w} - \psi^T\left[\frac{\partial R}{\partial w}\right]\right\}_I \delta w + \left\{\frac{\partial I^T}{\partial \mathcal{F}} - \psi^T\left[\frac{\partial R}{\partial \mathcal{F}}\right]\right\}_{II} \delta \mathcal{F}\end{aligned} \tag{6}$$

Choosing ψ to satisfy the adjoint equation

$$\left[\frac{\partial R}{\partial w}\right]^T \psi = \frac{\partial I}{\partial w} \tag{7}$$

the first term is eliminated, and we find that

$$\delta I = \mathcal{G}\delta \mathcal{F} \tag{8}$$

where

$$\mathcal{G} = \frac{\partial I^T}{\partial \mathcal{F}} - \psi^T\left[\frac{\partial R}{\partial \mathcal{F}}\right]$$

The advantage is that Eq. (8) is independent of δw, with the result that the gradient of I with respect to an arbitrary number of design variables can be determined without the need for additional flow-field evaluations. In the case that Eq. (4) is a partial-differential equation, the adjoint Eq. (7) is also a partial-differential equation and determination of the appropriate boundary conditions requires careful mathematical treatment.

In Ref. [114], Jameson derived the adjoint equations for transonic flows modeled by both the potential flow equation and the Euler equations. The theory was developed in terms of partial-differential equations, leading to an adjoint partial-differential equation. In order to obtain numerical solutions both the flow and the adjoint equations must be discretized. However, the control theory might be applied directly to the discrete flow equations which result from the numerical approximation of the flow equations by finite element, finite volume or finite difference procedures. This leads directly to a set of discrete adjoint equations with a matrix which is the transpose of the Jacobian matrix of the full set of discrete nonlinear flow equations. On a three-dimensional mesh with indices ijk, the individual adjoint equations may be derived by collecting together all the terms multiplied by the variation δw_{ijk} of the discrete flow variable w_{ijk}. The resulting discrete adjoint equations represent a possible discretization of the adjoint partial-differential equation. If these equations are solved exactly they can provide an exact gradient of the inexact cost function which results from the discretization of the flow equations. Moreover, the discrete adjoint equations derived directly from the discrete flow equations become very complicated when the flow equations are discretized with higher order upwind biased schemes using flux limiters. On the other hand any consistent discretization of the adjoint partial-differential equation will yield the exact gradient in the limit as the mesh is refined.

The discrete adjoint equations, whether they are derived directly or by discretization of the adjoint partial-differential equation, are linear. Therefore they could be solved by direct numerical inversion. In three-dimensional problems on a mesh with, say, n intervals in each coordinate direction, the number of unknowns is proportional to n^3 and the bandwidth to n^2. The complexity of direct inversion is proportional to the number of unknowns multiplied by the square of the bandwidth, resulting in a complexity proportional to n^7. The cost of direct inversion can thus become prohibitive as the mesh is refined, and it becomes more efficient to use iterative solution methods. Moreover, because of the similarity of the adjoint equations to the flow equations, the same iterative methods which have been demonstrated

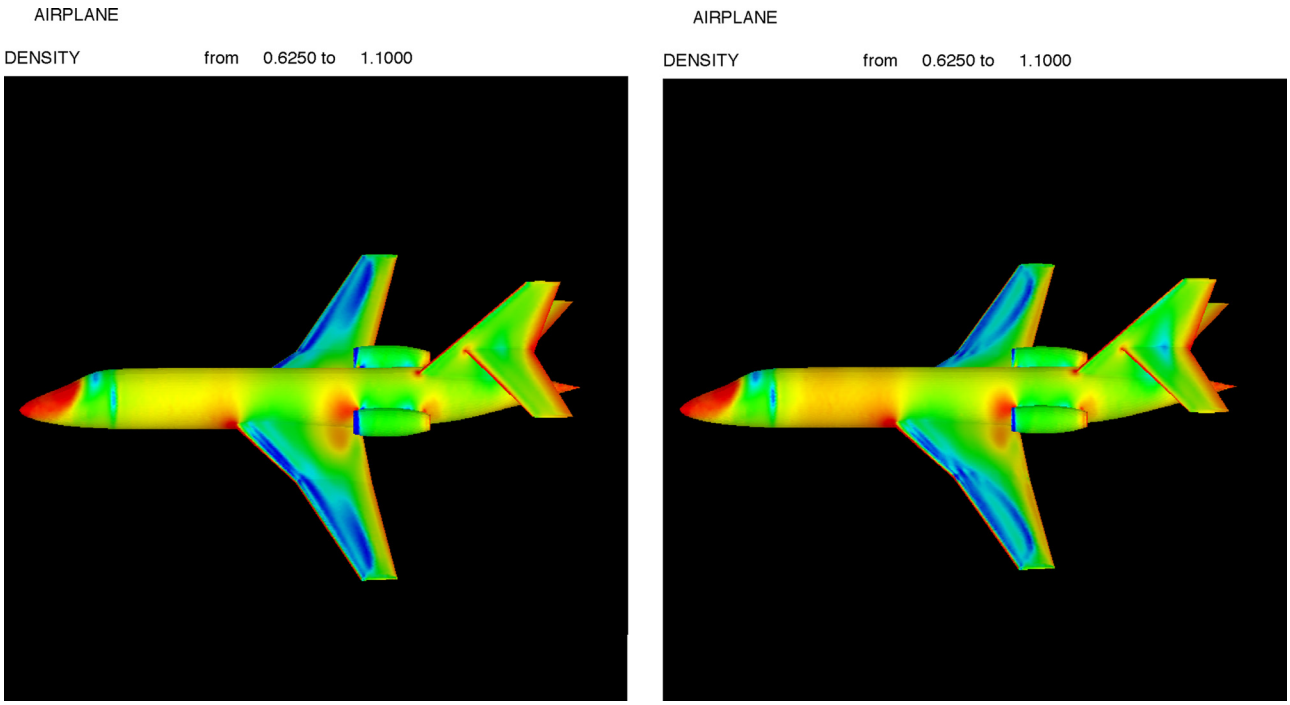

Fig. 3 Density contours on the surface of business jet: left original configuration—right optimized

to be efficient for the solution of the flow equations are efficient for the solution of the adjoint equations.

Studies of the use of control theory for optimum shape design of systems governed by elliptic equations were initiated by Pironneau [115]. The control theory approach to optimal aerodynamic design was first applied to transonic flow by Jameson [114,116–120]. He formulated the method for inviscid compressible flows with shock waves governed by both potential flow and the Euler equations [114]. Numerical results showing the method to be extremely effective for the design of airfoils in transonic potential flow were presented in Ref. [121], and for three-dimensional wing design using the Euler equations in Ref. [122]. Subsequently the method has been employed for the shape design of complex aircraft configurations [123,124], using a grid perturbation approach to accommodate the geometry modifications. The method has been used to support the aerodynamic design studies of several industrial projects, including the Beech Premier and the McDonnell Douglas MDXX and blended wing-body projects. The application to the MDXX is described in Ref. [118]. The experience gained in these industrial applications made it clear that the viscous effects cannot be ignored in transonic wing design, and the method has therefore been extended to treat the Reynolds averaged Navier–Stokes equations [120]. Adjoint methods have also been the subject of studies by a number of other authors, including Baysal and Eleshaky [125], Huan and Modi [126], Desai and Ito [127], Anderson and Venkatakrishnan [128], and Peraire and Elliot [129]. Ta'asan et al. [130], who have implemented a one shot approach in which the constraint represented by the flow equations is only required to be satisfied by the final converged solution. In their work, computational costs are also reduced by applying multigrid techniques to the geometry modifications as well as the solution of the flow and adjoint equations.

More recently, the continuous adjoint methods has been implemented on unstructured tetrahedral meshes. Figure 3 depicts the computed density contours of the original and optimized aircraft. It shows that the shock wave footprint is more diffuse in the optimized configuration, consistent with the fact that the computed drag has been reduced from 235 to 215 counts [131].

4 Conclusion and Future Challenges

Progress in both algorithms and computer hardware has evolved computational aerodynamics into an economical and indispensable tool for aerodynamic design. It has indeed become the main tool used in industry to carry out the initial phases of a design—conceptual and preliminary; while wind tunnel testing provides the final validation. The design of the wing planform, high-speed wing lines, wing tips, wing-body fairings, vertical tail is today carried out primarily via CFD. Furthermore, CFD provides an avenue for extending wind tunnel test results to flight Reynolds numbers. In spite of these successes, much remains to be achieved. On the numerical side, there remains the need both to improve the accuracy of computational simulations, and to assure known levels of accuracy. This will be crucial for CFD to become an acceptable tool in the certification process of new airframes, a goal that would greatly reduce the costs of bringing new aircrafts into service. Today, adjoint-based optimization techniques enable the aerodynamicist to optimize transonic wings for cruise condition. While they are not intended to replace the judgement and insight of the aircraft designers, they are a powerful enabling tool that allows the designers to focus their efforts on the creative aspects of aircraft design, by relieving them of the need to spend large amounts of time exploring small variations. The next challenge is the development of optimization techniques for off-design conditions, and for time-dependent flow. This will require advances in both numerical algorithms and modeling of highly separated turbulent flow. To meet this challenge, current efforts focus on the development of higher order accuracy methods based on spectral differences and on a discontinuous Galerkin approach, and on the development of well calibrated large eddy simulation (LES) models.

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