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Shape Inverse Design and Optimization for Three-Dimensional Aerodynamics

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SHAPE INVERSE DESIGN AND OPTIMIZATION FOR THREE-DIMENSIONAL AERODYNAMICS

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Abstract

A number of existing and emerging concepts for formulating methodologies applicable to automatic inverse design and optimization of arbitrary realistic three-dimensional aerodynamic configurations have been surveyed and compared. An attempt was made to classify the methods and to expose their major advantages and disadvantages. The existing flow-field analysis codes were found to be useful integral parts of all techniques surveyed. The methods for inverse aerodynamic shape design were found to be a potentially useful integral part of the general shape optimization. Similarly, different optimization and convergence acceleration algorithms were found to be potentially useful integral parts of the control theory (adjoint operator) based concepts that seem to be the most promising overall approach to the shape design optimization.

Introduction

A need for defining and solving inverse problems and performing multipoint and multidisciplinary optimization is becoming increasingly important in numerous areas of engineering. In general, engineering field problems are defined by the governing partial differential or integral equation(s), shape(s) and size(s) of the domain(s), boundary and initial conditions, material properties of the media contained in the field, and by internal sources and external forces or inputs.

Inverse problems in engineering disciplines dealing with field quantities can be classified[1] as:

1. Shape design inverse problems: determination of the shapes, sizes, and locations of the domains including multiply connected regions (shape determination, identification or optimization in acoustics, aerodynamics, electromagnetics, heat conduction, etc.; detection of voids and cracks).

2. Material properties inverse problems: determination of physical properties of the media modeled by the governing equation(s) since they form the coefficients in such equations.

3. Boundary value/initial value inverse problems: identification of the proper boundary conditions and/or initial conditions (tomographic problems involving x-rays, optics, thermal fields, etc.; determination of thermal boundary conditions in heat conduction).

4. Sources and forces inverse problems: determination of the unknown internal or external concentrated sources or inputs acting on the domain (structural dynamics modification and reconstruction, etc.).

5. Governing equation(s) inverse problems: inference of the equation(s) governing the variation of field quantities in physical problems that are presently described by inadequate analytical models.

The aerodynamic shape inverse design involves the ability to determine the shape of an aerodynamic configuration that will satisfy the governing flow-field equation(s) subject to specified surface pressure or velocity boundary conditions and certain geometric constraints.

The aerodynamic shape optimization involves the ability to determine the shape of an aerodynamic configuration that will satisfy the governing flow-field equation(s) subject to iteratively-adjusted surface pressure or velocity boundary conditions and certain flow-field or geometric constraints so that the global aerodynamic parameters (lift, drag, lift/drag, moment, etc.) are properly extremized. Relevant publications include conference proceedings[2-6], survey articles[7-9] and a new technical journal *Inverse Problems in Engineering*. The entire design technology is driven by the increased industrial demand for reduction of the design cycle time and minimization of the need for the costly *a posteriori* design modifications with the recognition that this technology is a key to maintaining international competitiveness.

This article will focus on classifying, briefly explaining and evaluating only these aerodynamic shape inverse design and optimization concepts that are applicable to three-dimensional (3-D) configurations and that are cost effective, reliable, easy to comprehend and implement, transportable and accurate.

Aerodynamic Shape Inverse Design

Stream-Function-Coordinate (SFC) Concept

It is well known[10] that 3-D inviscid compressible steady flows can be modeled with two stream functions,

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$\Psi(x,y,z)$ and $\Lambda(x,y,z)$. In the case of a typical 3-D flow-field analysis we are solving for the values of $\Psi(x,y,z)$ and $\Lambda(x,y,z)$ while treating x,y,z surface coordinates of the 3-D flight vehicle as known[11]. In the inverse shape design case we can derive two non-linear second order partial differential equations that treat the x-coordinate and the values of $\Psi(x,y,z)$ and $\Lambda(x,y,z)$ or their derivatives as known quantities on the yet unknown solid surface of the 3-D configuration[10,12-14]. Numerical solution of these two highly-coupled equations of the mixed type will give values of $y = y(x,\Psi,\Lambda)$ and $z = z(x,\Psi,\Lambda)$ for every 3-D streamline. Those streamlines that correspond to the specified surface values of $\Psi(x,y,z)$ and $\Lambda(x,y,z)$ are recognized as the desired 3-D aerodynamic configuration.

This inverse design method requires development of an entirely new code for the solution of the two Stream-Function-as-a-Coordinate (SFC) equations. The code converges very fast because it implicitly satisfies mass at every iteration step. It can be executed in either: a) analysis mode when Dirichlet boundary conditions for $\Psi(x,y,z)$ and $\Lambda(x,y,z)$ are specified at every surface point, or b) inverse design mode when Neumann boundary conditions are specified at every yet unknown surface point.

Despite its remarkable speed of execution, robustness and the fact that the entire field of 3-D streamlines is obtained as a by-product of the computation, the SFC concept has its serious disadvantages. It is not applicable to viscous flow models, suffers from the difficulties of the geometric multivaluedness of the stream functions, and is analytically singular at all the points where the Jacobian of transformation $\partial(\Psi,\Lambda,0)/\partial(x,y,z)$ becomes zero[10]. This occurs at every point where the x-component of the local velocity vector is zero which can happen at a number of points whose locations we do not know *a priori*. Consequently, the SFC method is recommended only for the inverse design of smooth 3-D configurations where preferably there are no stagnation points (3-D duct or where we are willing to neglect the designed shape in the vicinity of the leading and trailing edges. It is possible to localize the errors due to singularities of the transformation by reformulating the SFC in terms of the locally streamline-aligned Cartesian system s,n,m where s is the streamline-aligned coordinate. In this case the SFC formulation is singular at the stagnation lines which could be located in an *a priori* fashion and treated separately.

Elastic Membrane Motion Concept

Because of the large number of reliable and relatively-fast flow-field analysis codes in existence, the ultimate need of an aerodynamic designer is to utilize them in the inverse shape design and optimization process with preferably no modifications. Therefore, it would be logical to develop such user-friendly 3-D shape inverse design methods that can utilize any of the existing flow-field analysis codes as large subroutines, that is, it can call either a 3-D surface panel, or full potential, or Euler, or parabolized Navier-Stokes, or thin-layer Navier-Stokes, etc. flow-field analysis code treating them as a black box.

Parts of the surface of the aerodynamic flight vehicle that are desired to have a specified surface pressure distribution can be heuristically treated as elastic membranes. If each point of the membrane is loaded with a point-force, ΔC_p, that is proportional to the local difference between the computed, C_p^{calc}, and the specified, C_p^{spec}, coefficient of surface pressure, the membrane will iteratively deform until it assumes a steady position that experiences zero forcing function at each of the membrane points. Since this is a general non-physical concept for modeling the unsteady damped motion of the 3-D aerodynamic surface, any analytical expression governing damped motion of continuous surface will suffice. Garabedian and McFadden[15] suggested a simple second-order linear partial differential equation as such a model where ΔC_p is proportional to the local surface slopes and curvatures.

$$\beta_0 \frac{\partial \Delta n}{\partial t} + \beta_1 \frac{\partial^2 \Delta n}{\partial x \partial t} + \beta_2 \frac{\partial^2 \Delta n}{\partial y \partial t} + \beta_3 \frac{\partial^3 \Delta n}{\partial x^2 \partial t} + \beta_4 \frac{\partial^3 \Delta n}{\partial y^2 \partial t} = \beta_5 \Delta C_p \qquad (1)$$

Here, the unknowns are the displacements, Δn, of the aerodynamic surface in the direction locally normal to the surface. The time step Δt is arbitrary and may be set to a value of $\Delta t = 1.0$. If the surface grid point in question is on the upper surface, $\beta_5 = 1.0$, if on the lower surface, $\beta_5 = -1.0$. This partial differential equation is discretized using finite difference representations for the partial derivatives that leads to one penta-diagonal system or a sequence of two three-diagonal systems of algebraic equations that can readily be solved for the unknown normal surface modifications, Δn_i. This simple technique was successfully used to design isolated 3-D transonic supercritical wings[15] with a 3-D full potential code as the flow analysis module.. A simplified version of this concept (with Δz instead of Δn) was used to design engine nacelles[16] and wing-body configurations[17] engine. The method converges monotonically to a smooth shape even for a very irregular specified distribution of surface pressures and for a significantly wrong initial guess for the geometry.

Nevertheless, it has been observed in practice[18] and can be shown analytically[19] that the radius of convergence of the iterative matrix in the present formulation of this method depends on the non-linearity of the flow-field analysis module. This means that when using a progressively more nonlinear flow-field analysis module we will need between two and three orders of magnitude more analysis runs than when using a simple linear panel code. For example, in two-dimensional airfoil shape inverse design with this method utilizing a Navier-Stokes flow analysis code may require over ten thousand calls to the Navier-Stokes code[18]. This is obviously unacceptable for 3-D applications.

A worthwhile effort would be to investigate other analytical models governing the aerodynamic surface unsteady motion where the coefficients are treated as non-constant and are continuously optimized for the maximum convergence. Combining this simple technique with the indirect surface transpiration concept could make this method more economically acceptable.

Indirect Surface Transpiration Concept

This is definitely the simplest concept to comprehend and to implement for updating the surface geometry. It is based upon the objective of finding a configuration that satisfies two constraints: a) the zero velocity component normal to the final body surface, and b) the velocity component tangential to the final body surface that corresponds to the desired surface pressure distribution. The solution of the inverse (design) problem leads to a flow that corresponds to the prescribed tangential velocity components, v_t^{spec}, on the surface, but does not satisfy the zero normal velocity components at the surface. The computed normal velocity components are then used to modify the shape of the surface using a surface transpiration analogy. The new surface shape is predicted by treating the old surface as porous by fictitiously injecting the mass ($\rho\, v_n$) normal to the original surface so that the new surface becomes an updated stream surface. The local surface displacements, Δn, can be obtained from mass conservation equations for the quasi two-dimensional sections (stream tubes) of the flow-field bounded by the two consecutive cross sections of the body surface, the original surface shape and the unknown surface shape displaced locally by Δn. A crude extension of the formula for two-dimensional shape design can be written[20-22] as

$$(\Delta m)_{i-1,j}((\Delta n\,\rho\, v_t^{ave})_{i-1,j-1} + (\Delta n\,\rho\, v_t^{ave})_{i-1,j}) / 2$$
$$+(\Delta s)_{i,j-1}\,((\Delta m\,\rho\, v_n^{calc})_{i-1,j-1} + (\Delta m\,\rho\, v_n^{calc})_{i,j-1}) / 2$$
$$+(\Delta s)_{i,j}((\Delta m\,\rho\, v_n^{calc})_{i-1,j} + (\Delta m\,\rho\, v_n^{calc})_{i,j}) / 2$$
$$+(\Delta s)_{i,j-1}\,((\Delta n\,\rho\, v_m^{calc})_{i-1,j-1} + (\Delta n\,\rho\, v_m^{calc})_{i,j-1}) / 2$$
$$+(\Delta s)_{i,j}\,((\Delta n\,\rho\, v_m^{calc})_{i-1,j} + (\Delta n\,\rho\, v_m^{calc})_{i,j}) / 2$$
$$= (\Delta m)_{i,j}((\Delta n\,\rho\, v_t^{ave})_{i,j-1} + (\Delta n\,\rho\, v_t^{ave})_{i,j}) / 2 \qquad (2)$$

where $(\Delta m)_{i,j}$ is the old j-distance between the surface points (i,j) and (i,j-1), $(\Delta s)_{i,j}$ is the old i-distance between the surface points (i,j) and (i-1,j),while

$$(v_t^{ave})_{i-1,j-1} = ((v_t^{calc})_{i-1,j-1} + (v_t^{spec})_{i-1,j-1}) / 2 \qquad (3)$$

with similar expressions for $(v_t^{ave})_{i-1,j}$, $(v_t^{ave})_{i,j-1}$, $(v_t^{ave})_{i,j}$ and $(v_m^{ave})_{i-1,j-1}$, $(v_m^{ave})_{i,j-1}$, $(v_m^{ave})_{i-1,j}$ and $(v_m^{ave})_{i-1,j}$. Starting from a stagnation line where $(\Delta n)_{i-1,j} = 0.0$ and $(\Delta n)_{i-1,j+1} = 0.0$, separate updating of the pressure surface and the suction surface can be readily performed by solving for $(\Delta n)_{i,j}$ and $(\Delta n)_{i,j+1}$ from a bi-diagonal system given by the combination of equations (2) and (3). With the classical transpiration concept, surface normal velocities can be computed using any potential flow solver including a fast and accurate surface panel flow analysis code. Nevertheless, the indirect surface transpiration method works quite satisfactory in conjunction with Euler and even Navier-Stokes equations barring any shock waves or flow separation. During the repetitive surface updating using this method, the updated surface can develop a progressively-increasing degree of oscillation. This can be eliminated by periodically smoothing the updated surface with a least-squares surface fitting algorithm. It should be pointed out that since this formulation implies an *a priori* knowledge of the specified tangential surface velocity component direction, this approach is not as readily applicable to fully 3-D design as it seems.

Direct Surface Transpiration Concept

A more direct method of utilizing the transpiration concept is similar to the more common direct flow analysis problem, but the manner of treating boundary conditions on surfaces is different[23]. For example, in the flow analysis with Navier-Stokes equations, the no-slip condition is imposed at the surface, that is U = V = W = 0. In the inverse shape design, the surface pressure distribution, which is obtained from the specified pressure coefficient distribution, is enforced iteratively together with U = W = 0. This can be done readily in any existing Navier-Stokes flow analysis code. This will result in the contravariant velocity vector component, V, becoming non-zero at the surface. Hence, the surface will have to move regularly with iterations or time steps until the convergence is reached, that is, until V = 0 is satisfied on the final surface configuration. This is essentially a surface-transpiration concept where the surface movement velocity along the η-grid line that originates from the surface could be chosen to equal V. This will require that the computational grid be regenerated with each update of the surface. Thus, the aerodynamic parameters need to be transfered between old and new grid points by an accurate 3-D interpolation.

If the code is executed in a time-accurate mode, this method will provide for a time-accurate motion of the solid boundaries. This implies that with this concept it is possible to determine the correct instantaneous values of local swelling and contraction of a "smart" material coating on the surface thus providing for an essentially steady surface pressure distribution in an unsteady flow. The need for the smart or continuously-adaptable aerodynamic shape design is expected to grow rapidly.

Characteristic Boundary Condition Concept

A less heuristic, thus more reliable and faster, is the inverse shape design method based on the solid boundary characteristic boundary conditions. The correct number and types of boundary conditions for a hyperbolic system of partial differential equations can be determined by analyzing eigenvalues and the corresponding eigenvectors of the system in each coordinate direction separately. This approach to boundary condition treatment is called characteristic boundary conditions[24] since it suggests one-dimensional application of certain Riemann invariants at the boundaries. For example, in a 3-D duct flow, if the speed is locally subsonic at the exit, we will be able to compute all flow variables at the exit based on the information from the interior points except for one variable that we will have to specify at the exit. Often, this variable is the exit pressure. In a flow-field analysis case, this would represent a problem since we do not know *a priori* the appropriate pressure distribution on the exit plane. But, if the same characteristic boundary condition procedure is applied in the direction normal to the solid wall and if the desired pressure distribution is specified on the wall, this method of enforcing the boundary conditions at the wall will result in non-zero velocities at the wall which can be used to update the wall shape. The general concept follows.

The Euler equations for 3-D compressible unsteady flows expressed in non-conservative form and cast in a boundary-conforming, non-orthogonal, curvilinear (ξ,η,ζ) coordinate system are

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{Q}}{\partial \xi} + \mathbf{B}\frac{\partial \mathbf{Q}}{\partial \eta} + \mathbf{C}\frac{\partial \mathbf{Q}}{\partial \zeta} = \mathbf{H} \qquad (4)$$

where $\mathbf{Q} = (\rho, \rho u, \rho v, \rho w, \rho e_o)$ is the transposed vector of the conservative solution variables and $\mathbf{H}$ is the vector of source terms (non-conservative body forces). This system can be transformed into

$$\frac{\partial \tilde{\mathbf{Q}}}{\partial \tau} + \tilde{\mathbf{B}}\frac{\partial \tilde{\mathbf{Q}}}{\partial \eta} + \tilde{\mathbf{D}} = 0 \qquad (5)$$

where $\tilde{\mathbf{Q}} = (\rho\ p\ u\ v\ w)$ is the transposed vector of the non-conservative primitive variables. Eigenvalues of $\tilde{\mathbf{B}}$ are

$$V - c\,(\eta_x^2 + \eta_y^2 + \eta_z^2)^{1/2},$$

$$V, V, V, V + c\,(\eta_x^2 + \eta_y^2 + \eta_z^2)^{1/2}) \qquad (6)$$

where $V = \eta_t + (\eta_x u + \eta_y v + \eta_z w)$ and the local speed of sound is defined as $c = (\gamma\, p / \rho)^{1/2}$. If the η-grid lines are emanating from the 3-D aerodynamic configuration, we can have several situations. If $0 < V < c\,(\eta_x^2 + \eta_y^2 + \eta_z^2)^{1/2}$, one eigenvalue is negative requiring a pressure boundary condition to be specified at that surface point. If $-c\,(\eta_x^2 + \eta_y^2 + \eta_z^2)^{1/2} < V < 0$, four eigenvalues will be negative requiring pressure, velocity ratio $u/(u^2 + v^2 + w^2)^{1/2}$, total pressure and total temperature to be specified at that surface point. If $V < -c\,(\eta_x^2 + \eta_y^2 + \eta_z^2)^{1/2}$, all five eigenvalues will be negative requiring pressure, velocity ratios $u/(u^2 + v^2 + w^2)^{1/2}$ and $v/(u^2 + v^2 + w^2)^{1/2}$, total pressure and total temperature to be specified at that surface point. This method has been shown[25,26] to converge very quickly for transonic two-dimensional airfoil shape design analyzed by compressible flow Euler equations. It requires modifications to solid-wall boundary condition subroutines in the existing flow-field analysis codes. The method is conceptually applicable to the inverse design of arbitrary 3-D configurations although no such attempts have been reported yet. Similar to the direct transpiration concept, if the Euler code is executed in a time-accurate mode, the specified unsteady solid wall characteristic boundary conditions will provide for a time-accurate motion of the solid boundaries which is highly attractive for the design of "smart" aerodynamic configurations. This concept is not applicable to viscous flow analysis codes since velocity components at the solid wall are zero.

Geometry-Velocity Perturbation Concept

Numerous sensitivity analysis formulations for aerodynamic shape design that have been published recently[27-32] as an integral part of the multidisciplinary design optimization effort[33] have an impressive predecessor in the works of Bristow[34,20]. He used the boundary element method to analyze potential flow around the initial and consecutively perturbed configurations by utilizing 3-D source and dipole distributions on each flat surface panel. The local surface tangential and normal velocity vector components due to the linear combination of the free stream at an angle α and the surface singularities are

$$V_{Ti}^{calc} = \cos(\Theta_i - \alpha) + A_{\sigma ij}\,\sigma_j + A_{\gamma ij}\,\gamma_j \qquad (7)$$

$$V_{Ni}^{calc} = -\sin(\Theta_i - \alpha) + B_{\sigma ij}\,\sigma_j + B_{\gamma ij}\,\gamma_j \qquad (8)$$

If the initial geometry is perturbed by adding to each local surface panel angle Θ_i an arbitrary angle $\delta\Theta_i$ then the velocity component at the midpoint of surface panel i will also be perturbed as follows

$$V_{Ti}^{calc} + \delta V_{Ti}^{calc} = \cos(\Theta_i + \delta\Theta_i - \alpha)$$
$$+ (A_{\sigma ij} + \delta A_{\sigma ij})(\sigma_j + \delta\sigma_j)$$
$$+ (A_{\gamma ij} + \delta A_{\gamma ij})(\gamma_j + \delta\gamma_j) \qquad (9)$$

with a similar expression resulting from equation (8). By subtracting equations (7) and (8) from these expressions, neglecting higher order terms in δ and expressing perturbations of the geometric influence coefficient matrices $\delta A_{\sigma ij}$, $\delta A_{\gamma ij}$, $\delta B_{\sigma ij}$ and $\delta B_{\gamma ij}$ as functions of $\delta\Theta_i$, the resulting equations linearly relating the perturbations in the surface velocity vector components and the surface panel angles are obtained as

$$\delta V_{Ti}^{calc} = A_{\Theta ij}\,\delta\Theta_i + A_{\sigma ij}\,\delta\sigma_j + A_{\gamma ij}\,\delta\gamma_j \qquad (10)$$

with the similar expressions for other velocity components. These equations and the analogous expressions for the perturbations at edges of the surface panels can be combined with the 3-D boundary element flow analysis method to give

$$\delta V_{Ti}^{calc} = \overset{*}{A}_{\Theta ij}\,\delta\Theta_j \qquad (11)$$

with the similar expressions for the perturbations of other velocity components where coefficient matrices like $\overset{*}{A}_{\Theta ij}$ are functions of the unperturbed geometry only. The equations (11) correspond to a first order expansion about the flow-field of an arbitrary body. In the case of a flat plate these equations approach the classical linearized potential flow theory. The global least squares error E between the specified and the calculated surface tangential velocities at panel midpoints and endpoints is

$$E = \sum^{npan-1} \left\{ \sum^{npan} \left[\Delta S_i \,(V_{Ti}^{spec} - V_{Ti}^{calc})^2\right] \right.$$

$$\left. + \sum^{npan-1} \left[\Delta S_l \,(V_{Tl}^{spec} - V_{Tl}^{calc})^2\right] \right\} \qquad (12)$$

where ΔS_i are the panel lengths. Finally, δE, with the help of equations (11) and (12), can be expressed as a direct function of the local geometry perturbations $\delta\Theta_j$.

This inverse design method is exceptionally robust since it converges even with initial configurations that are significantly different from their final shapes. It is also accurate and computationally efficient since it is based on the fast and versatile boundary element (surface panel) technique. It typically requires between 3-7 inverse design cycles to fully converge. The main drawback of this design concept is that it is tightly linked to the incompressible inviscid potential flow analysis code which can account for viscous effects only via often tedious and unreliable viscous-inviscid coupling. Similarly, only linearized compressibility effects can be introduced via Prandtl-Glauert coordinate transformation making this design concept unsuitable for the inverse design of 3-D transonic configurations.

Integro-Differential Equation Concept

An impressively fast and versatile 3-D shape inverse design algorithm has been developed by Takanashi[35]. It can accept any available 3-D flow-field analysis code as a large subroutine to analyze the flow around the intermediate 3-D configurations. The configurations are updated using a fast integro-differential formulation. Specifically, a velocity potential perturbation $\phi(x,y,z)$ around an initial 3-D configuration $z^{+/-}(x,y)$ can be obtained with, for example, a Navier-Stokes code[36] where the subscripts +/- refer to the upper and lower surfaces of the flight vehicle. In addition, if a differentially small perturbation $\Delta\phi(x,y,z)$ is introduced in the 3-D transonic small perturbation equation, the result is

$$\frac{\partial^2\Delta\phi}{\partial x^2} + \frac{\partial^2\Delta\phi}{\partial y^2} + \frac{\partial^2\Delta\phi}{\partial z^2}$$

$$= \frac{1}{V_{oo}}\frac{\partial}{\partial x}\left(\frac{1}{2}\left(\frac{\partial\phi}{\partial x} + \frac{\partial\Delta\phi}{\partial x}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2\right) = \frac{1}{V_{oo}}\frac{\partial\Gamma}{\partial x} \qquad (13)$$

where x,y,z have been scaled via Prandtl-Glauert transformation, V_{oo} is the free stream magnitude, while

$$\frac{\partial\phi(x,y,+/-0)}{\partial x} = -\frac{V_{oo}}{2}C_{p+/-}(x,y) \qquad (14)$$

$$\frac{\partial\Delta\phi(x,y,+/-0)}{\partial x} = -\frac{(1+\kappa)\,M\,a_{oo}^2}{2\,(1 - M\,a_{oo}^2)}\left(C_{p+/-}^{spec} - C_{p+/-}^{calc}\right) \qquad (15)$$

Here, M is the local Mach number and a_{oo} is the free stream speed of sound. Flow tangency condition is then

$$\frac{\partial\Delta\phi(x,y,+/-0)}{\partial z} = V_{oo}\,\frac{\partial\Delta z_{+/-}(x,y)}{\partial x} \qquad (16)$$

Since $\frac{\partial\Delta\phi(x,y,+/-0)}{\partial z}$ can be obtained from equation (13), the 3-D geometry is readily updated from

$$\Delta z_{+/-}(x,y) =$$

$$\frac{1}{2}\int_0^x \frac{\partial[\Delta z_+(x,y) + \Delta z_-(x,y)]}{\partial x}\,dx$$

$$\pm\frac{1}{2}\int_0^x \frac{\partial[\Delta z_+(x,y) - \Delta z_-(x,y)]}{\partial x}\,dx \qquad (17)$$

Since equation (13) is linear, it can be reformulated using Green's theorem as an integro-differential equation. The Γ term on the right hand side of equation (13) would require volume integration which can be avoided if Γ is prescribed as smoothly decreasing away from the 3-D flight vehicle surface[36,37] where it is known. Then, the problem can be very efficiently solved using 3-D boundary element method. This inverse shape design concept has been successfully applied to a variety of planar wings[35,38] and wing-body configurations including the H-II Orbiting Plane with winglets[36] where 3-D flow-field analysis codes were of the full potential, Euler and Navier-Stokes type. The method typically requires 10-30 flow analysis runs with an arbitrary flow solver and as many solutions of the linearized integro-differential equation.

Aerodynamic Shape Optimization Concepts

The common drawback of all inverse shape design methods is that they create designs that are not optimal in any sense even at the design conditions. At off design, these configurations often perform quite poorly except when C_p^{spec} is provided by an experienced aerodynamics expert. This implies a need for expensive, highly-specialized personnel which is not the general trend in industry. Also, when using inverse shape design methods it is impossible to generate a 3-D aerodynamic configuration that simultaneously satisfies the specified surface distribution of flow variables, manufacturing constraints (leading edge radius, trailing edge closure, trailing edge included angle, magnitude and location of the relative maximum thickness, etc.), utilization constraints (cockpit or cabin size, engine inlet area, etc.) and achieve the best global aerodynamic performance (overall aerodynamic drag minimized, lift and lift/drag ratio maximized, etc.). Consequently, the designer should use an adequate global optimization algorithm that can utilize any available flow-field analysis code without changes and efficiently optimize the overall aerodynamic characteristics of the 3-D flight vehicle subject to the finite set of desired constraints and global flight operating conditions. The constraints could be purely geometrical or they can be of the overall aerodynamic nature (minimize overall drag for the given values of flight speed, angle of attack and overall lift force, etc.). The size and shape of the mathematical space that contains all the design variables (all surface coordinates) is very large and complex in a typical 3-D case. To find a global minimum of such a space requires a sophisticated numerical optimization algorithm that avoids local minimums, honors the specified constraints and stays within the feasible design domain.

There are many optimization algorithms capable of performing these tasks, although they require a large number of function evaluations, that is, they need to call the time-consuming aerodynamic flow-field analysis code many times. Despite this, the optimization algorithms are still often misused to minimize the difference between the specified and the computed surface flow data - a task that is significantly more economical when accomplished with any of the simple inverse shape design algorithms. Thus, only these optimization algorithms that require minimum number of calls to the flow-field analysis code will be realistic candidates for the 3-D aerodynamic shape optimization .

The most serious drawback of the brute force application of the gradient search optimization in 3-D aerodynamics is that the computing costs increase nonlinearly with the growing number of design variables[39]. Therefore, only when it is possible to use trivially simple and fast flow-field analysis codes like Newton impact theory in hypersonics[40] could we afford for the ideal situation where each surface grid point on the 3-D optimized configuration is allowed to move independently. Otherwise, we are forced to work with a relatively small number of the design variables by performing parametrization of either the 3-D surface geometry[41] or the 3-D specified surface pressure field[42]. The optimizer then needs to optimize the coefficients in these polynomials. The most plausible choices like cubic splines[43]. Chebyshev and Fourier polynomials[40] are not accurate and advisable, because they become excessively oscillatory with the increasing number of terms. Moreover, when perturbing any of the coefficients in such a polynomial, the entire 3-D shape will change. Since it is absolutely necessary to constrain and sometimes not allow motion of the particular parts of the 3-D surface of a flight vehicle, the most promising choices for the 3-D parametrization appear to be Bezier curves[44], local analytical surface patches[45] and local polynomial basis functions[22].

Constrained Gradient Search Algorithms

Standard gradient search optimization algorithms[39], if the function space is large and disproportionately scaled, almost certainly have an abundance of local minimums. These minimums are very hard to negotiate even by switching the objective function formulation[46] or consecutive spline fitting and interpolation of the unidirectional search step parameter[46]. A comparative analysis of gradient-based search optimization algorithms[47,27] confirms that more economical techniques are possible. Single-cycle optimization[48] is one such possibility where an optimizer is used on each updated configuration even before the flow-field has fully converged to the new geometry. An optimal aerodynamic shape is then found by optimally weighing each of the number of feasible configurations that can be obtained using inverse design methods. Hence, this optimization approach guarantees that the final configuration will be realistically shaped and manufacturable, although the range of geometric parameters to be optimized is limited by the extreme members of the original family of configurations.

Genetic Evolution Optimization Algorithms

Besides a wide variety of the gradient-based optimization algorithms, truly remarkable results were obtained in the late seventies using an evolution type genetic algorithm[49]. Although the standard genetic algorithm (GA) is computationally quite expensive since it requires a large number of calls to the flow-field analysis code, the robustness of this algorithm and the ease of its implementation have created a recently renewed interest in applying it for aerodynamic shape design[50-53]. Nevertheless, all of the examples in these publications involve two-dimensional airfoil shape optimization with a small number of design variables that form a relatively compact function space. Solution of such optimization problems would be considerably more efficient when using more common gradient search algorithms. Moreover, none of the examples in these publications attempt to treat constrained optimization which represents the most difficult problem for a typical GA algorithm[54]. The classical GA can handle constraints on the design variables, but it is not inherently capable of handling constraint functions. Most of the recent publications involving GA and aerodynamic shape optimization have involved problems posed in such a way as to eliminate constraint functions, or to penalize the cost function when a constraint is violated. These treatments of constraints reduce the chance of arriving at the global minimum.

One of the most attractive features of the GA is its remarkable robustness since it is not a gradient-based search method. Thus, it is especially suitable for the types of problems where the sensitivity derivatives might be discontinuous which is often the case in 3-D aerodynamic optimization. The number of cost function evaluations per design iteration of a GA does not depend on the number of design variables. Rather, it depends on the size of the initial population. The GA is also exceptional at avoiding local minima, because it tests possible designs over a large domain in the design variable space.

The GA has proven itself to be an effective and robust optimization tool for large variable-set problems if the cost function evaluations are very cheap to perform. Nevertheless, in the field of 3-D aerodynamic shape optimization we are faced with the more difficult situation where each cost function evaluation is extremely costly and the number of the design variables is relatively large. GA will require large memory if large number of design variables are used. Consequently, the brute force application of the standard GA to 3-D aerodynamic shape design optimization is economically unjustifiable. A combination of the GA and a gradient search optimization or the GA and an inverse design method might be an advisable way to proceed.

Combined Inverse Design and Optimization

The unique feature of this concept is that it offers the most economical approach to constrained aerodynamic shape optimization. It consists of two phases. In the first phase it parametrizes the initial C_p^{spec} distribution and optimizes it without calling a flow analysis code. For this purpose, the use is made of extremely efficient approximate relations linking the integrated surface pressure distribution and object's maximum thickness[42], specified location of the flow transition points and the aerodynamic drag from any of the classical boundary layer solutions, etc. The optimization of the few coefficients of, for example, Bezier parametrization of the C_p^{spec} curves[55] can be performed reliably and economically with any of the optimization algorithms since the total number of optimization variables is small, the design space does not have an excessive number of local minimums and the sensitivity derivatives do not have discontinuities. This combined design procedure easily accepts constraints such as the desired slopes of C_p^{spec} curves at the leading and trailing edges, maximum value of C_p^{spec}, a condition that the C_p^{spec} values on the suction surface are never smaller than on the pressure surface, etc. The resulting optimized C_p^{spec} distribution will correspond to the minimum drag, specified lift and other desired aerodynamic features of a yet unknown 3-D optimized configuration.

The second phase of this 3-D shape design concept utilizes the optimized C_p^{spec} distribution and any of the fast inverse design algorithms to find the corresponding 3-D configuration. This design methodology seems to require minimum development time due to the use of existing optimization codes, flow analysis codes and preferably those inverse design codes that can accept any flow analysis code as a large subroutine. Hence, this method is capable of creating 3-D optimized constrained aerodynamic configurations at the cost slightly higher than required by a 3-D inverse shape design.

Optimization Using Sensitivity Derivatives

It is often desirable to have a capability to predict the behavior of the inputs to an arbitrary system by relating the outputs to the inputs via a sensitivity derivative matrix, while treating the system as a black box. The sensitivity derivative matrix can be used for the purpose of controlling the system outputs or to achieve an optimized constrained design that depends on the system outputs[27-33]. The objective is to generate approximations of the infinite dimensional sensitivities and to transfer these approximate derivatives to the optimizer together with the approximate function evaluations. The control variables are then updated with the sensitivity derivatives which are the gradients of the cost function with respect to the control variables. The general concepts for the sensitivity analysis can be summarized[27] as follows. The entire system of governing flow-field governing equations after discretizations results in a system of non-linear algebraic equations

$$\mathbf{R}(\mathbf{Q}(\mathbf{D}), \mathbf{X}(\mathbf{D}), \mathbf{D}) = 0 \qquad (18)$$

where $\mathbf{X}$ is the computational grid and $\mathbf{D}$ is the vector of design variables. Hence

$$\frac{d\mathbf{R}}{d\mathbf{D}} = \frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\frac{d\mathbf{Q}}{d\mathbf{D}} + \frac{\partial \mathbf{R}}{\partial \mathbf{X}}\frac{d\mathbf{X}}{d\mathbf{D}} + \frac{\partial \mathbf{R}}{\partial \mathbf{D}} = 0 \qquad (19)$$

Similarly, aerodynamic output functions are defined as

$$\mathbf{F} = \mathbf{F}(\mathbf{Q}(\mathbf{D}), \mathbf{X}(\mathbf{D}), \mathbf{D}) \qquad (20)$$

Hence

$$\frac{d\mathbf{F}}{d\mathbf{D}} = \frac{\partial \mathbf{F}}{\partial \mathbf{Q}}\frac{d\mathbf{Q}}{d\mathbf{D}} + \frac{\partial \mathbf{F}}{\partial \mathbf{X}}\frac{d\mathbf{X}}{d\mathbf{D}} + \frac{\partial \mathbf{F}}{\partial \mathbf{D}} \qquad (21)$$

System (19) is solved for the sensitivity derivatives of the field variables, $\frac{dQ}{dD}$, which are then substituted in the system (21) in order to obtain the sensitivity derivatives of the desired aerodynamic outputs, $\frac{dF}{dD}$. This approach is typically used if the dimension of **F** is greater than that of **D**. Otherwise, it is more economical to avoid solving for $\frac{dQ}{dD}$ by using an adjoint operator approach where a linear system

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right)^T \mathbf{A} + \left(\frac{\partial \mathbf{F}}{\partial \mathbf{Q}}\right)^T = 0 \tag{22}$$

must be solved first for **A** which is a discrete adjoint variable matrix associated with the aerodynamic output functions, **F**. Consequently, the aerodynamic output derivatives of interest are computed from

$$\frac{d\mathbf{F}}{d\mathbf{D}} = \left(\mathbf{A}^T \frac{\partial \mathbf{R}}{\partial \mathbf{X}}\frac{d\mathbf{X}}{d\mathbf{D}} + \mathbf{A}^T \frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right) + \frac{\partial \mathbf{F}}{\partial \mathbf{X}}\frac{d\mathbf{X}}{d\mathbf{D}} + \frac{\partial \mathbf{F}}{\partial \mathbf{D}} \tag{23}$$

This quasi-analytical approach to computing sensitivity derivatives is more economical than when evaluating the derivatives using finite differencing.

Optimization Using Newton Flow Solvers

In the gradient-search optimization approach the flow analysis code must be called at least once for each design variable in order to compute the gradient of the objective function during each optimization cycle. Since each call to the analysis code is very expensive, such approach to design is justified only if an inadequately small number of design variables is used. In the case of a 3-D design, this is hardly justifiable even if one uses 3-D surface geometry parametrization, thus severely constraining possible 3-D optimal configurations.

The most promising recent development in the aerodynamic shape design optimization is a method that treats the governing system of partial differential equations as constraints, while treating locations of all surface grid points as design variables[56]. This approach eliminates the need for geometry parametrization using shape functions to define changes in the geometry. Since fluid dynamic variables are treated here as the design variables, this method allows for rapid computation of partial derivatives of the objective function with respect to the design variables. This approach is straightforward to comprehend and efficient to implement in Newton-type direct flow analysis algorithms where solutions of the equations for $\frac{dQ}{dD}$ or **A** amount to a simple back-substitution.

Nevertheless, the classical Newton iteration algorithm is practically impossible to implement for 3-D aerodynamic analysis codes because of its excessive memory requirements when performing direct LU factorization of the coefficient matrix. Instead of using an exact Newton algorithm in the flow-analysis code, it is more cost effective to use a quasi-Newton iterative formulation or an incremental iterative strategy[32] given in the form

$$-\frac{\partial \tilde{\mathbf{R}}}{\partial \mathbf{Q}}\, \Delta\left(\frac{d\mathbf{Q}}{d\mathbf{D}}\right) = \left(\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right)^n = \frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\left(\frac{d\mathbf{Q}}{d\mathbf{D}}\right)^n + \frac{\partial \mathbf{R}}{\partial \mathbf{X}}\frac{d\mathbf{X}}{d\mathbf{D}} + \frac{\partial \mathbf{R}}{\partial \mathbf{D}} \tag{24}$$

$$\left(\frac{d\mathbf{Q}}{d\mathbf{D}}\right)^{n+1} = \left(\frac{d\mathbf{Q}}{d\mathbf{D}}\right)^n + \Delta\left(\frac{d\mathbf{Q}}{d\mathbf{D}}\right) \quad ; \; n = 1, 2, 3, \ldots \tag{25}$$

where $\frac{\partial \tilde{\mathbf{R}}}{\partial \mathbf{Q}}$ could be any fully-converged numerical approximation of the exact Jacobian matrix.

Adjoint Operator (Control Theory) Concepts

With the increasing number of variables that need to be optimized, the discrete function space containing the optimization variables tends towards a continuous function space for which it is possible to use a global analytical formulation (an adjoint system) instead of the local discretized formulation (gradient search and genetic evolution algorithms). If the governing system of partial differential equations is large and significantly non-linear, then the control theory (adjoint operator) approach is more appropriate than the other two approaches. Published results of 3-D elbow diffuser shape optimization using the adjoint operator approach and incompressible laminar flow Navier-Stokes equations[57-59] suggest that a typical design takes between five and twelve 3-D analysis solutions involving both the Navier-Stokes and the adjoint system. Similar total effort (5-25 solutions of the two systems) was reported[60-62] for 3-D transonic isolated wing design. These results dispel earlier reservations that adjoint operator approach formulations might not be computationally efficient since they involve the solution of an additional set of adjoint equations and several more interface equations. This could be compared with several hundreds and even thousands of flow analysis runs when using a genetic algorithm or a typical gradient search algorithm.

If the adjoint system is different from the original system, a significant effort needs to be invested in separately coding the two systems. If the adjoint system is almost the same as the original governing system, the numerical algorithms for the two systems are practically the same and the entire approach could be implemented more readily using the existing CFD analysis software.

One drawback of the adjoint operator (control theory) approach is that it requires the derivation of an entirely new system of partial differential equations in terms of some non-physical adjoint variables and specification of their boundary conditions. This is not a trivial undertaking since there are many ways to derive the adjoint system and some additional partial differential equations and their boundary conditions coupling the original system and the adjoint system. An additional drawback of the entire adjoint operator approach is that it does not allow for flow separation and that it suffers from the local minimums like most of the gradient search optimizers. The complexity of the entire adjoint operator formulation makes it difficult to comprehend and implement. Nevertheless, once it is fully debugged, the adjoint operator concept seems to offer the most economical method for 3-D aerodynamic shape design and optimization.

Convergence Acceleration and Reliability Enhancement

Reduction of total computing time required by iterative algorithms for numerical integration of Navier-Stokes equations for 3-D, compressible, turbulent flows with heat transfer is an important aspect in the making of existing and future analysis codes widely acceptable as main components of design tools. Reliability of flow-field analysis codes is an equally important item especially when varying input parameters over a wide range of values. Although a variety of methods have been tried, it remains one of the most challenging tasks to develop and extensively verify new concepts that will guarantee substantial reduction of computing time over a wide range of grid qualities (clustering, skewness, etc.), flow-field parameters (Mach numbers, Reynolds numbers, etc.), types and sizes of systems of partial differential equations (elliptic, parabolic, hyperbolic, etc.). While a number of methods are capable of reducing the total number of iterations required to reach the converged solution, they require more time per iteration so that the effective reduction in the total computing time is often negligible.

The main commonality of the more prominent methods for acceleration of iterative convergence rates (preconditioning[63], multigrid[64], GMRES[65]) is that they all experience loss of their ability to reduce the computing time on highly-clustered non-orthogonal grids that are unavoidable for 3-D aerodynamic configurations and high Reynolds number turbulent flows. The new sensitivity-based minimal residual (SBMR) method[66] and its 3-D analogy[65] have been shown to successfully reduce the computational effort by 50% even for highly-clustered non-orthogonal grids. The general formulation of this acceleration method is applicable to both explicit and implicit iteration schemes. Hence, it should be possible to apply these new acceleration methods in conjunction with the other acceleration methods (preconditioning, multigridding, etc.) to explore the possibilities for a cumulative acceleration effect.

In the case of optimization methods based on sensitivity analysis, the main difficulty is to make the evaluation of the derivatives less difficult and more reliable. A worthwhile effort is to research further on use of the automatic differentiation (ADIFOR) based on a chain-rule for evaluating the derivatives of the functions defined by flow analysis code with respect to its input variables[67,68,31]. This approach still needs to be made more computationally efficient

An equally worthwhile effort is to further research the "one shot" method that carefully combines the adjoint operator approach and the multigrid method[69]. This algorithm optimizes the control variables on coarse grids, thus eliminating costly repetitive flow analysis on fine grids during each optimization cycle. The entire shape optimization should be ideally accomplished in one application of the full multigrid flow solver[70].

Conclusions

After comparing a variety of methods applicable to inverse design and optimization of 3-D aerodynamic shapes it can be concluded that: a) combination of inverse design and optimization will be an attractive approach in the immediate future, b) brute force application of gradient-based and genetic evolution optimizers is uneconomical for realistic 3-D problems, c) sensitivity-based optimization methods will be superceeded by the adjoint operator formulations, d) automatic differentiation and one-shot methods should be further researched. Particular emphasis should be placed on integrating the 3-D grid generation, convergence acceleration, shape inverse design and shape optimization codes into a unified aerodynamic design module that is highly robust, versatile, computationally efficient and transportable integral part of the 3-D multidisciplinary design and optimization.

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