Aerodynamic Shape Optimization Techniques Based On Control Theory

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OBJECTIVE OF COMPUTATIONAL AERODYNAMICS

1. Capability to predict the flow past an airplane in different flight regimes
   - take off
   - cruise (transonic)
   - flutter
2. Interactive design calculations to allow immediate improvement
3. Automatic design optimization

AERODYNAMIC DESIGN METHODS

1945 LIGHTHILL (Conformal Mapping, Incompressible Flow)
1965 NIEUWLAND (Hodograph, Power Series)
1970 GARABEDIAN - KORN (Hodograph, Complex Characteristics)
1974 BOERSTOEL (Hodograph)
1974 TRENEN (Potential Flow, Dirichlet Boundary Conditions)
1977 HENNE (3-D Potential Flow, Based on FLO22)
1985 VOLPE-MELNIK (2-D Potential Flow, Based on FLO36)
1979 GARABEDIAN - McFADDEN (Potential Flow, Neuman Boundary Conditions, Iterated Mapping)
1976 SOBIECZI (Fictitious Gas)
1979 DRELA - GILES (2-D Euler Equations, Streamline Coordinates, Newton Iteration)

LIGHTHILL'S METHOD

Design Profile C for Specified Surface speed q_t.

Let a profile C be conformally mapped to a circle by

$$\log \frac{dz}{d\sigma} = \sum \frac{C_n}{\sigma^n}$$

$$\log \frac{ds}{d\theta} + i\left(\alpha - \theta - \frac{\pi}{2}\right) = \sum (a_n \cos(n\theta) + b_n \sin(n\theta) + i \sum (b_n \cos(n\theta) - a_n \sin(n\theta))$$

Where

$$q = \frac{\nabla \phi}{h} \quad , \quad h = \frac{dz}{d\sigma}$$

and

$$\phi = \left(r + \frac{1}{r}\right) \cos\theta + \frac{\Gamma}{2\pi}\theta \qquad \text{is known}$$

On C set $q = q_t$

$$\rightarrow \frac{ds}{d\theta} = \frac{\phi_\theta}{q_t} \rightarrow a_n \ , \ b_b$$

CONSTRAINTS WITH LIGHTHILL'S METHOD

To preserve q_∞

$$c_0 = 0$$

Also, integration around a circuit gives

$$\Delta z = \oint \frac{dz}{d\sigma} d\sigma = 2\pi i c_1$$

Closure $\rightarrow c_1 = 0$

Thus,

$$\int \log(q_t) d\theta = 0$$

$$\int \log(q_t) \cos(\theta) d\theta = 0$$

$$\int \log(q_t) \sin(\theta) d\theta = 0$$

DIRICHLET METHOD by VOLPE-MELNIK

Assume a conformal mapping to a circle.

Then transonic potential flow satisfies

$$\frac{\partial \rho \phi_\theta}{\partial \theta} + r \frac{\partial r \rho \phi_r}{\partial r} = 0 \tag{1}$$

Where

$$\rho = \left[1 + \frac{\gamma - 1}{2} M_\infty^2 \left(1 - q^2\right)\right)^{\frac{1}{\gamma - 1}} \quad , \quad q = \frac{\nabla \phi}{h} \quad , \quad h = \left|\frac{dz}{dr}\right|$$

On C integrate the target speed to obtain

$$\phi = \int q_t ds$$

DIRICHLET METHOD (cont.)

Solve equation (1) with a Dirichlet boundary condition

$$\frac{\partial \phi}{\partial n} = v \neq 0 \qquad , \qquad \text{at} \quad r = 1 \qquad \rightarrow \delta\alpha = \frac{v}{u}$$

Correct the mapping and iterate

CONSTRAINTS WITH DIRICHLET METHOD

LIGHTHILL'S constraints still apply.

Therefore allow freedom in the target speed

$$q_t = p_0 f_0(s) + p_1 f_1(\theta) + p_2 f_2(\theta)$$

Where $f_0(s)$ represents the desired speed distribution,

$f_1(\theta)$ and $f_2(\theta)$ are distributions selected to allow adjustment for closure,

and p_0, p_1, p_2 are free parameters.

NEUMANN METHOD by GARABEDIAN- McFADDEN

Assume an initial mapping $h^{(0)} = \left|\frac{dz}{dr}\right|$ and solve

$$\frac{\partial \rho \phi_\theta}{\partial \theta} + r\frac{\partial r \rho \phi_r}{\partial r} = 0 \qquad (2)$$

for ϕ. Then on C

$$q^{(0)} = \frac{\phi_\theta}{h^{(0)}}$$

Adjust h so that $q = q_t$

$$\frac{h^{(1)}}{h^{(0)}} = \frac{q^{(0)}}{q_t}$$

Iterate

$$\log\left(h^{(n+1)}\right) = \log\left(h^{(n+1)}\right) - \log\left(\frac{q^{(n)}}{q_t}\right)$$

NEUMANN METHOD (cont.)

In the low Mach number limit this reduces to Lighthill's method.

If q_t is smooth and q has a shock, then the shape correction has a corner.

CONTROL THEORY APPROACH TO THE DESIGN PROBLEM

Define a cost function

$$I = \frac{1}{2} \int_{\mathcal{B}} (p - p_t)^2 \; d\mathcal{B}$$

or

$$I = \frac{1}{2} \int_{\mathcal{B}} (q - q_t)^2 \; d\mathcal{B}$$

The surface shape is now treated as the control, which is to be varied to minimize I, subject to the constraint that the flow equations are satisfied in the domain $\mathcal{D}$

CHOICE OF DOMAIN

ALTERNATIVES

1. Variable computational domain – Free boundary problem
2. Transformation to a fixed computational domain – Control via the transformation function.

EXAMPLES

1. 2-D via Conformal mapping with potential flow
2. 2-D via Conformal mapping with Euler equations
3. 3-D Sheared Parabolic Coordinates with Euler Equation
4. . . .

FORMULATION OF THE CONTROL PROBLEM

Suppose that the surface of the body is expressed by an equation

$$f(\underline{x}) = 0$$

Vary f to $f + \delta f$ and find δI.

If we can express

$$\delta I = \int_{\mathcal{B}} g \delta f d\mathcal{B} = (g, \delta f)_{\mathcal{B}}$$

Then we can recognize g as the gradient $\frac{\partial I}{\partial f}$.

Choose a modification

$$\delta f = -\lambda g$$

Then to first order

$$\delta I = -\lambda (g, g)_{\mathcal{B}} < 0$$

FORMULATION OF THE CONTROL PROBLEM (cont.)

In the presence of constraints project g into the admissible trial space.

Accelerate by the conjugate gradient method.

TRADITIONAL APPROACH TO DESIGN OPTIMIZATION

The simplest approach to optimization is to define the geometry through a set of design parameters, which may, for example, be the weights α_i applied to a set of shape functions $b_i(x)$ so that the shape is represented as

$$f(x) = \sum \alpha_i b_i(x).$$

Then a cost function I is selected. The sensitivities $\frac{\partial I}{\partial \alpha_i}$ may now be estimated by making a small variation $\delta\alpha_i$ in each design parameter in turn and recalculating the flow to obtain the change in I. Then

$$\frac{\partial I}{\partial \alpha_i} \approx \frac{I(\alpha_i + \delta\alpha_i) - I(\alpha_i)}{\delta\alpha_i}.$$

The gradient vector $\frac{\partial I}{\partial \alpha}$ may now be used to determine a direction of improvement.

The simplest procedure is to make a step in the negative gradient direction by setting

$$\alpha^{n+1} = \alpha^n - \lambda \delta \alpha,$$

so that to first order

$$I + \delta I = I - \frac{\partial I^T}{\partial \alpha} \delta \alpha = I - \lambda \frac{\partial I^T}{\partial \alpha} \frac{\partial I}{\partial \alpha}.$$

DISADVANTAGES

The main disadvantage of this approach is the need for a number of flow calculations proportional to the number of design variables to estimate the gradient. The computational costs can thus become prohibitive as the number of design variables is increased.

GENERAL FORMULATION OF THE ADJOINT APPROACH TO OPTIMAL DESIGN

The progress of the design procedure is measured in terms of a cost function

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

where w are the flow-field variables and $\mathcal{F}$ is the location of the boundary.

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. [1]

[1] 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

The governing equations of the flow field

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

which express the dependence of w and $\mathcal{F}$ are introduced as a constraint within the flow-field domain $\mathcal{D}$. Then δw is determined from the equation

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

Next, introducing a Lagrange Multiplier ψ, we have

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

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

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

Once equation (8) is established, an improvement can be made with a shape change

$$\delta\mathcal{F} = -\lambda\mathcal{G}$$

where λ is positive, and small enough that the first variation is an accurate estimate of δI. The variation in the cost function then becomes

$$\delta I = -\lambda\mathcal{G}^T\mathcal{G} < 0.$$

ADVANTAGES

- Equation (8) is independent of δw. Hence, the gradient of I with respect to an arbitrary number of design variables can be determined without the need for additional flow-field evaluations.
- The computational cost of a single design cycle is roughly equivalent to the cost of two flow solutions since the the adjoint problem has similar complexity.
- When the number of design variables becomes large, the computational efficiency of the control theory approach over traditional approach, which requires direct evaluation of the gradients by individually varying each design variable and recomputing the flow field, becomes compelling.

AIRFOIL DESIGN FOR POTENTIAL FLOW USING CONFORMAL MAPPING

Consider the case of two-dimensional compressible inviscid flow. In the absence of shock waves, an initially irrotational flow will remain irrotational, and we can assume that the velocity vector $\mathbf{q}$ is the gradient of a potential ϕ.

In the presence of weak shock waves this remains a fairly good approximation.

Let p, ρ, c, and M be the pressure, density, speed-of-sound, and Mach number q/c. Then the potential flow equation is

$$\nabla \cdot (\rho \nabla \phi) = 0, \tag{9}$$

where the density is given by

$$\rho = \left\{ 1 + \frac{\gamma - 1}{2} M_\infty^2 \left(1 - q^2 \right) \right\}^{\frac{1}{(\gamma - 1)}}, \tag{10}$$

while

$$p = \frac{\rho^\gamma}{\gamma M_\infty^2}, \quad c^2 = \frac{\gamma p}{\rho}. \tag{11}$$

Here M_∞ is the Mach number in the free stream, and the units have been chosen so that p and q have a value of unity in the far field.

Suppose that the domain D exterior to the profile C in the z-plane is conformally mapped on to the domain exterior to a unit circle in the σ-plane.

Let R and θ be polar coordinates in the σ-plane, and let r be the inverted radial coordinate $\frac{1}{R}$. Also let h be the modulus of the derivative of the mapping function

$$h = \left| \frac{dz}{d\sigma} \right|. \tag{12}$$

Now the potential flow equation becomes

$$\frac{\partial}{\partial \theta}\left(\rho \phi_\theta\right) + r\frac{\partial}{\partial r}\left(r\rho\phi_r\right) = 0 \;\text{ in } D, \tag{13}$$

where the density is given by equation (10), and the circumferential and radial velocity components are

$$u = \frac{r\phi_\theta}{h}, \quad v = \frac{r^2\phi_r}{h}, \tag{14}$$

while

$$q^2 = u^2 + v^2. \tag{15}$$

The condition of flow tangency leads to the Neumann boundary condition

$$v = \frac{1}{h}\frac{\partial \phi}{\partial r} = 0 \text{ on } C. \tag{16}$$

In the far field, the potential is given by an asymptotic estimate, leading to a Dirichlet boundary condition at $r = 0$.

Suppose that it is desired to achieve a specified velocity distribution q_d on C.

Introduce the cost function

$$I = \frac{1}{2}\int_C (q - q_d)^2 \, d\theta,$$

DESIGN PROBLEM

The design problem is now treated as a control problem where the control function is the mapping modulus h, which is to be chosen to minimize I subject to the constraints defined by the flow equations (9–16).

A modification δh to the mapping modulus will result in variations $\delta\phi$, δu, δv, and $\delta\rho$ to the potential, velocity components, and density. The resulting variation in the cost will be

$$\delta I = \int_C (q - q_d)\ \delta q\, d\theta, \tag{17}$$

where, on C, $q = u$. Also,

$$\delta u = r\frac{\delta\phi_\theta}{h} - u\frac{\delta h}{h},\quad \delta v = r^2\frac{\delta\phi_r}{h} - v\frac{\delta h}{h},\quad \frac{\partial\rho}{\partial u} = -\frac{\rho u}{c^2},\quad \frac{\partial\rho}{\partial v} = -\frac{\rho v}{c^2}.$$

It follows that $\delta\phi$ satisfies

$$L\delta\phi = -\frac{\partial}{\partial\theta}\left(\rho M^2 \phi_\theta \frac{\delta h}{h}\right) - r\frac{\partial}{\partial r}\left(\rho M^2 r \phi_r \frac{\delta h}{h}\right)$$

where

$$L \equiv \frac{\partial}{\partial\theta}\left\{\rho\left(1-\frac{u^2}{c^2}\right)\frac{\partial}{\partial\theta} - \frac{\rho u v}{c^2} r\frac{\partial}{\partial r}\right\} + r\frac{\partial}{\partial r}\left\{\rho\left(1-\frac{v^2}{c^2}\right) r\frac{\partial}{\partial r} - \frac{\rho u v}{c^2}\frac{\partial}{\partial\theta}\right\}. \tag{18}$$

Then, if ψ is any periodic differentiable function which vanishes in the far field,

$$\int_D \frac{\psi}{r^2} L\,\delta\phi\,dS = \int_D \rho M^2 \boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\psi\frac{\delta h}{h}\,dS, \tag{19}$$

where dS is the area element $r\,dr\,d\theta$, and the right hand side has been integrated by parts.

Now we can augment equation (17) by subtracting the constraint (19).

The auxiliary function ψ then plays the role of a Lagrange multiplier. Thus,

$$\begin{aligned}\delta I &= \int_C (q - q_d)\, q \frac{\delta h}{h}\, d\theta - \int_C \delta\phi \frac{\partial}{\partial\theta}\left(\frac{q - q_d}{h}\right) d\theta \\ &\quad - \int_D \frac{\psi}{r^2} L\delta\phi\, dS + \int_D \rho M^2 \boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}\psi \frac{\delta h}{h}\, dS.\end{aligned}$$

Now suppose that ψ satisfies the adjoint equation

$$L\psi = 0 \;\text{ in } D \tag{20}$$

with the boundary condition

$$\frac{\partial\psi}{\partial r} = \frac{1}{\rho}\frac{\partial}{\partial\theta}\left(\frac{q - q_d}{h}\right) \quad \text{on } C. \tag{21}$$

Then, integrating by parts,

$$\int_D \frac{\psi}{r^2} L\delta\phi \, dS = -\int_C \rho\psi_r\delta\phi \, d\theta,$$

and

$$\begin{aligned} \delta I &= -\int_C (q - q_d)\, q \frac{\delta h}{h} \, d\theta \\ &\quad + \int_D \rho M^2 \boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}\psi \frac{\delta h}{h} \, dS. \end{aligned} \tag{22}$$

Here the first term represents the direct effect of the change in the metric, while the area integral represents a correction for the effect of compressibility. When the second term is deleted the method reduces to a variation of Lighthill's method.

Equation (22) can be further simplified to represent δI purely as a boundary integral. Set

$$\log \frac{dz}{d\sigma} = \mathcal{F} + i\beta,$$

where

$$\mathcal{F} = \log \left| \frac{dz}{d\sigma} \right| = \log h,$$

and

$$\delta\mathcal{F} = \frac{\delta h}{h}.$$

Then $\mathcal{F}$ satisfies Laplace's equation

$$\Delta\mathcal{F} = 0 \text{ in } D,$$

and if there is no stretching in the far field, $\mathcal{F} \to 0$. Also $\delta\mathcal{F}$ satisfies the same conditions.

Introduce another auxiliary function P which satisfies

$$\Delta P = \rho M^2 \nabla\psi \cdot \nabla\psi \text{ in } D, \tag{23}$$

and

$$P = 0 \text{ on } C.$$

Then, the area integral in equation (22) is

$$\int_D \Delta P\, \delta\mathcal{F}\, dS = \int_C \delta\mathcal{F} \frac{\partial P}{\partial r}\, d\theta - \int_D P \Delta\, \delta\mathcal{F}\, dS,$$

and finally

$$\delta I = \int_C \mathcal{G}\, \delta\mathcal{F}\, d\theta,$$

where $\mathcal{F}_c$ is the boundary value of $\mathcal{F}$, and

$$\mathcal{G} = \frac{\partial P}{\partial r} - (q - q_d)\, q. \tag{24}$$

This suggests setting

$$\delta\mathcal{F}_c = -\lambda\mathcal{G}$$

so that if λ is a sufficiently small positive quantity

$$\delta I = -\int_C \lambda\mathcal{G}^2\, d\theta < 0.$$

Arbitrary variations in $\mathcal{F}$ cannot, however, be admitted. The condition that $\mathcal{F} \to 0$ in the far field, and also the requirement that the profile should be closed, imply constraints which must be satisfied by $\mathcal{F}$ on the boundary C. Suppose that $\log\left(\frac{dz}{d\sigma}\right)$ is expanded as a power series

$$\log\left(\frac{dz}{d\sigma}\right) = \sum_{n=o}^{\infty} \frac{c_n}{\sigma^n}, \tag{25}$$

where only negative powers are retained, because otherwise $\left(\frac{dz}{d\sigma}\right)$ would become unbounded for large σ. The condition that $\mathcal{F} \to 0$ as $\sigma \to \infty$ implies

$$c_o = 0.$$

Also, the change in z on integration around a circuit is

$$\Delta z = \int \frac{dz}{d\sigma}\, d\sigma = 2\pi i\, c_1,$$

so the profile will be closed only if

$$c_1 = 0.$$

In order to satisfy these constraints, we can project $\mathcal{G}$ onto the admissible subspace for $\mathcal{F}_c$ by setting

$$c_o = c_1 = 0. \tag{26}$$

Then the projected gradient $\tilde{\mathcal{G}}$ is orthogonal to $\mathcal{G} - \tilde{\mathcal{G}}$, and if we take

$$\delta \mathcal{F}_c = -\lambda \tilde{\mathcal{G}},$$

it follows that to first order

$$\begin{aligned} \delta I &= -\int_C \lambda \mathcal{G} \tilde{\mathcal{G}}\, d\theta = -\int_C \lambda \left(\tilde{\mathcal{G}} + \mathcal{G} - \tilde{\mathcal{G}} \right) \mathcal{G}\, d\theta \\ &= -\int_C \lambda \tilde{\mathcal{G}}^2\, d\theta < 0. \end{aligned}$$

If the flow is subsonic, this procedure should converge toward the desired speed distribution.

If, however, the flow is transonic, one must allow for the appearance of shock waves in the trial solutions, even if q_d is smooth. Then $q - q_d$ is not differentiable.

This difficulty can be circumvented. Consider

$$I = \frac{1}{2}\int_C \left(\lambda_1 \mathcal{Z}^2 + \lambda_2 \left(\frac{d\mathcal{Z}}{d\theta}\right)^2\right)\, d\theta, \tag{27}$$

where λ_1 and λ_2 are parameters, and the periodic function $\mathcal{Z}(\theta)$ satisfies the equation

$$\lambda_1 \mathcal{Z} - \frac{d}{d\theta}\lambda_2 \frac{d\mathcal{Z}}{d\theta} = q - q_d. \tag{28}$$

Then,

$$\begin{aligned} \delta I &= \int_C \left(\lambda_1 \mathcal{Z}\,\delta\mathcal{Z} + \lambda_2 \frac{d\mathcal{Z}}{d\theta}\frac{d}{d\theta}\,\delta\mathcal{Z}\right)\, d\theta \\ &= \int_C \mathcal{Z}\left(\lambda_1\,\delta\mathcal{Z} - \frac{d}{d\theta}\lambda_2 \frac{d}{d\theta}\,\delta\mathcal{Z}\right)\, d\theta = \int_C \mathcal{Z}\,\delta q\, d\theta. \end{aligned}$$

Thus, $\mathcal{Z}$ replaces $q - q_d$ in the previous formulas, and if one modifies the boundary condition (21) to

$$\frac{\partial \psi}{\partial r} = \frac{1}{\rho} \frac{\partial}{\partial \theta} \left(\frac{\mathcal{Z}}{h} \right) \quad \text{on } C, \tag{29}$$

the formula for the gradient becomes

$$\mathcal{G} = \frac{\partial P}{\partial r} - \mathcal{Z} q \tag{30}$$

instead of equation (24).

Smoothing can also be introduced directly in the descent procedure by choosing $\delta\mathcal{F}_c$ to satisfy

$$\delta\mathcal{F}_c - \frac{\partial}{\partial\theta}\beta\frac{\partial}{\partial\theta}\,\delta\mathcal{F}_c = -\lambda\mathcal{G}, \tag{31}$$

where β is a smoothing parameter. Then to first order

$$\begin{aligned}\int \mathcal{G}\,\delta\mathcal{F} &= -\frac{1}{\lambda}\int\left(\delta\mathcal{F}_c^2 - \delta\mathcal{F}_c\frac{\partial}{\partial\theta}\beta\frac{\partial}{\partial\theta}\,\delta\mathcal{F}_c\right)\,d\theta \\ &= -\frac{1}{\lambda}\int\left(\delta\mathcal{F}_c^2 + \beta\left(\frac{\partial}{\partial\theta}\,\delta\mathcal{F}_c\right)^2\right)\,d\theta < 0.\end{aligned}$$

FINAL DESIGN PROCEDURE

Choose an initial profile and corresponding mapping function $\mathcal{F}$. Then:

1. Solve the flow equations (9–16) for ϕ, u, v, q, ρ.
2. Solve the ordinary differential equation (28) for $\mathcal{Z}$.
3. Solve the adjoint equation (18 and 20) or ψ subject to the boundary condition (29).
4. Solve the auxiliary Poisson equation (23) for P.
5. Evaluate $\mathcal{G}$ by equation (30)
6. Correct the boundary mapping function $\mathcal{F}_c$ by $\delta\mathcal{F}_c$ calculated from equation (31), projected onto the admissible subspace defined by (26).
7. Return to step 1.

DESIGN USING THE EULER EQUATIONS

Denote the Cartesian coordinates and velocity components by x_1, x_2, x_3 and u_1, u_2, u_3, and use the convention that summation over $i = 1$ to 3 is implied by a repeated index i. Then, the three-dimensional Euler equations may be written as

$$\frac{\partial w}{\partial t} + \frac{\partial f_i}{\partial x_i} = 0 \quad \text{in } D, \tag{32}$$

where

$$w = \left\{ \begin{array}{c} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{array} \right\}, \quad f_i = \left\{ \begin{array}{c} \rho u_i \\ \rho u_i u_1 + p\delta_{i1} \\ \rho u_i u_2 + p\delta_{i2} \\ \rho u_i u_3 + p\delta_{i3} \\ \rho u_i H \end{array} \right\} \tag{33}$$

and δ_{ij} is the Kronecker delta function. Also,

$$p = (\gamma - 1)\,\rho\left\{E - \frac{1}{2}\left(u_i^2\right)\right\}, \tag{34}$$

and

$$\rho H = \rho E + p \tag{35}$$

where γ is the ratio of the specific heats.

Consider a transformation to coordinates ξ_1, ξ_2, ξ_3 where

$$K_{ij} = \left[\frac{\partial x_i}{\partial \xi_j}\right], \quad J = \det\left(K\right), \quad K_{ij}^{-1} = \left[\frac{\partial \xi_i}{\partial x_j}\right],$$

and

$$Q = JK^{-1}.$$

The elements of Q are the coefficients of K, and in a finite volume discretization they are just the face areas of the computational cells projected in the x_1, x_2, and x_3 directions.

Also introduce scaled contravariant velocity components as

$$U_i = Q_{ij} u_j.$$

The Euler equations can now be written as

$$\frac{\partial W}{\partial t} + \frac{\partial F_i}{\partial \xi_i} = 0 \quad \text{in } D, \tag{36}$$

where

$$W = Jw,$$

and

$$F_i = Q_{ij} f_j = \begin{bmatrix} \rho U_i \\ \rho U_i u_1 + Q_{i1} p \\ \rho U_i u_2 + Q_{i2} p \\ \rho U_i u_3 + Q_{i3} p \\ \rho U_i H \end{bmatrix}.$$

Assume now that the new computational coordinate system conforms to the wing in such a way that the wing surface B_W is represented by $\xi_2 = 0$.

Then the flow is determined as the steady state solution of equation (36) subject to the flow tangency condition

$$U_2 = 0 \quad \text{on } B_W. \tag{37}$$

At the far field boundary B_F, conditions are specified for incoming waves, as in the two-dimensional case, while outgoing waves are determined by the solution.

The weak form of the Euler equations for steady flow can be written as

$$\int_{\mathcal{D}} \frac{\partial \phi^T}{\partial \xi_i} F_i d\mathcal{D} = \int_{\mathcal{B}} n_i \phi^T F_i d\mathcal{B}, \tag{38}$$

where the test vector ϕ is an arbitrary differentiable function and n_i is the outward normal at the boundary. If a differentiable solution w is obtained to this equation, it can be integrated by parts to give

$$\int_{\mathcal{D}} \phi^T \frac{\partial F_i}{\partial \xi_i} d\mathcal{D} = 0.$$

Suppose now that it is desired to control the surface pressure by varying the wing shape. For this purpose, it is convenient to retain a fixed computational domain and then, variations in the shape result in corresponding variations in the mapping derivatives defined by K. Introduce the cost function

$$I = \frac{1}{2} \int\int_{B_W} (p - p_d)^2 \, d\xi_1 d\xi_3,$$

where p_d is the desired pressure. The design problem is now treated as a control problem where the control function is the wing shape, which is to be chosen to minimize I subject to the constraints defined by the flow equations (36–). A variation in the shape will cause a variation δp in the pressure and consequently a variation in the cost function

$$\delta I = \int\int_{B_W} (p - p_d) \, \delta p \;\; d\xi_1 d\xi_3. \tag{39}$$

Since p depends on w through the equation of state (34–35), the variation δp can be determined from the variation δw. Define the Jacobian matrices

$$A_i = \frac{\partial f_i}{\partial w}, \qquad C_i = Q_{ij} A_j. \tag{40}$$

The weak form of the equation for δw in the steady state becomes

$$\int_{\mathcal{D}} \frac{\partial \phi^T}{\partial \xi_i} \delta F_i d\mathcal{D} = \int_{\mathcal{B}} (n_i \phi^T \delta F_i) d\mathcal{B},$$

where

$$\delta F_i = C_i \delta w + \delta Q_{ij} f_j,$$

which should hold for any differential test function ϕ. This equation may be added to the variation in the cost function, which may now be written as

$$\delta I = \int\int_{B_W} (p - p_d)\, \delta p \;\; d\xi_1 d\xi_3 - \int_{\mathcal{D}} \left(\frac{\partial \psi^T}{\partial \xi_i} \delta F_i \right) d\mathcal{D} + \int_{\mathcal{B}} \left(n_i \psi^T \delta F_i \right) d\mathcal{B}. \tag{41}$$

On the wing surface B_W, $n_1 = n_3 = 0$. Thus, it follows from equation (37) that

$$\delta F_2 = \begin{bmatrix} 0 \\ Q_{21}\delta p \\ Q_{22}\delta p \\ Q_{23}\delta p \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \delta Q_{21} p \\ \delta Q_{22} p \\ \delta Q_{23} p \\ 0 \end{bmatrix}. \tag{42}$$

Since the weak equation for δw should hold for an arbitrary choice of the test vector ϕ, we are free to choose ϕ to simplify the resulting expressions. Therefore we set $\phi = \psi$, where the costate vector ψ is the solution of the adjoint equation

$$\frac{\partial \psi}{\partial t} - C_i^T \frac{\partial \psi}{\partial \xi_i} = 0 \quad \text{in } D. \tag{43}$$

At the outer boundary incoming characteristics for ψ correspond to outgoing characteristics for δw. Consequently one can choose boundary conditions for ψ such that

$$n_i \psi^T C_i \delta w = 0.$$

Then, if the coordinate transformation is such that δQ is negligible in the far field, the only remaining boundary term is

$$-\int\int_{B_W} \psi^T \delta F_2 \, d\xi_1 d\xi_3.$$

Thus, by letting ψ satisfy the boundary condition,

$$Q_{21}\psi_2 + Q_{22}\psi_3 + Q_{23}\psi_4 = (p - p_d) \quad \text{on } B_W, \tag{44}$$

we find finally that

$$\delta I = -\int_{\mathcal{D}} \frac{\partial \psi^T}{\partial \xi_i} \delta Q_{ij} f_j d\mathcal{D} - \int\int_{B_W} (\delta Q_{21}\psi_2 + \delta Q_{22}\psi_3 + Q_{23}\psi_4) \, p \, d\xi_1 d\xi_3. \tag{45}$$

THE NAVIER STOKES EQUATIONS

$$\frac{\partial w}{\partial t} + \frac{\partial f_i}{\partial x_i} = \frac{\partial f_{vi}}{\partial x_i} \quad \text{in } \mathcal{D}, \tag{46}$$

where the state vector w, inviscid flux vector f and viscous flux vector f_v are described respectively by

$$w = \left\{ \begin{array}{c} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{array} \right\}, \; f_i = \left\{ \begin{array}{c} \rho u_i \\ \rho u_i u_1 + p\delta_{i1} \\ \rho u_i u_2 + p\delta_{i2} \\ \rho u_i u_3 + p\delta_{i3} \\ \rho u_i H \end{array} \right\}, \quad f_{vi} = \left\{ \begin{array}{c} 0 \\ \sigma_{ij}\delta_{j1} \\ \sigma_{ij}\delta_{j2} \\ \sigma_{ij}\delta_{j3} \\ u_j \sigma_{ij} + k\frac{\partial T}{\partial x_i} \end{array} \right\}. \tag{47}$$

In these definitions, ρ is the density, u_1, u_2, u_3 are the Cartesian velocity components, E is the total energy and δ_{ij} is the Kronecker delta function.

The pressure is determined by the equation of state

$$p = (\gamma - 1)\,\rho \left\{ E - \frac{1}{2}\,(u_i u_i) \right\},$$

and the stagnation enthalpy is given by

$$H = E + \frac{p}{\rho},$$

where γ is the ratio of the specific heats. The viscous stresses may be written as

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \delta_{ij} \frac{\partial u_k}{\partial x_k}, \tag{48}$$

where μ and λ are the first and second coefficients of viscosity. The coefficient of thermal conductivity and the temperature are computed as

$$k = \frac{c_p \mu}{Pr}, \quad T = \frac{p}{R\rho}. \tag{49}$$

It is also useful to consider a transformation to the computational coordinates (ξ_1,ξ_2,ξ_3) defined by the metrics

$$K_{ij} = \left[\frac{\partial x_i}{\partial \xi_j}\right], \quad J = \det\left(K\right), \quad K_{ij}^{-1} = \left[\frac{\partial \xi_i}{\partial x_j}\right].$$

The Navier-Stokes equations can then be written in computational space as

$$\frac{\partial\left(Jw\right)}{\partial t} + \frac{\partial\left(F_i - F_{vi}\right)}{\partial \xi_i} = 0 \quad \text{in } \mathcal{D}, \tag{50}$$

where the inviscid and viscous flux contributions are now defined with respect to the computational cell faces by $F_i = S_{ij} f_j$ and $F_{vi} = S_{ij} f_{vj}$, and the quantity $S_{ij} = J K_{ij}^{-1}$ represents the projection of the ξ_i cell face along the x_j axis. In obtaining equation (50) we have made use of the property that

$$\frac{\partial S_{ij}}{\partial \xi_i} = 0\ . \tag{51}$$

FORMULATION OF THE OPTIMAL DESIGN PROBLEM FOR THE NAVIER STOKES EQUATIONS

Suppose that the performance is measured by a cost function

$$I = \int_{\mathcal{B}} \mathcal{M}(w, S)\, d\mathcal{B}_\xi + \int_{\mathcal{D}} \mathcal{P}(w, S)\, d\mathcal{D}_\xi,$$

containing both boundary and field contributions where $d\mathcal{B}_\xi$ and $d\mathcal{D}_\xi$ are the surface and volume elements in the computational domain. In general, $\mathcal{M}$ and $\mathcal{P}$ will depend on both the flow variables w and the metrics S defining the computational space. In the case of a multi-point design the flow variables may be separately calculated for several different conditions of interest.

The design problem is now treated as a control problem where the boundary shape represents the control function, which is chosen to minimize I subject to the constraints defined by the flow equations (50).

A shape change produces a variation in the flow solution δw and the metrics δS which in turn produce a variation in the cost function

$$\delta I = \int_{\mathcal{B}} \delta \mathcal{M}(w, S)\, d\mathcal{B}_\xi + \int_{\mathcal{D}} \delta \mathcal{P}(w, S)\, d\mathcal{D}_\xi, \qquad (52)$$

with

$$\begin{aligned} \delta \mathcal{M} &= [\mathcal{M}_w]_I\, \delta w + \delta \mathcal{M}_{II}, \\ \delta \mathcal{P} &= [\mathcal{P}_w]_I\, \delta w + \delta \mathcal{P}_{II}, \end{aligned} \qquad (53)$$

where we continue to use the subscripts I and II to distinguish between the contributions associated with the variation of the flow solution δw and those associated with the metric variations δS. Thus $[\mathcal{M}_w]_I$ and $[\mathcal{P}_w]_I$ represent $\frac{\partial \mathcal{M}}{\partial w}$ and $\frac{\partial \mathcal{P}}{\partial w}$ with the metrics fixed, while $\delta \mathcal{M}_{II}$ and $\delta \mathcal{P}_{II}$ represent the contribution of the metric variations δS to $\delta \mathcal{M}$ and $\delta \mathcal{P}$.

In the steady state, the constraint equation (50) specifies the variation of the state vector δw by

$$\frac{\partial}{\partial \xi_i} \delta \left(F_i - F_{vi} \right) = 0. \tag{54}$$

Here δF_i and δF_{vi} can also be split into contributions associated with δw and δS using the notation

$$\begin{aligned} \delta F_i &= [F_{iw}]_I \, \delta w + \delta F_{iII} \\ \delta F_{vi} &= [F_{viw}]_I \, \delta w + \delta F_{viII}. \end{aligned} \tag{55}$$

The inviscid contributions are easily evaluated as

$$[F_{iw}]_I = S_{ij} \frac{\partial f_j}{\partial w}, \qquad \delta F_{iII} = \delta S_{ij} f_j.$$

The details of the viscous contributions are complicated by the additional level of derivatives in the stress and heat flux terms and will be derived.

Multiplying by a co-state vector ψ, which will play an analogous role to the Lagrange multiplier, and integrating over the domain produces

$$\int_{\mathcal{D}} \psi^T \frac{\partial}{\partial \xi_i} \delta \left(F_i - F_{vi}\right) = 0. \tag{56}$$

If ψ is differentiable this may be integrated by parts to give

$$\int_{\mathcal{B}} n_i \psi^T \delta \left(F_i - F_{vi}\right) d\mathcal{B}_\xi - \int_{\mathcal{D}} \frac{\partial \psi^T}{\partial \xi_i} \delta \left(F_i - F_{vi}\right) d\mathcal{D}_\xi = 0. \tag{57}$$

Since the left hand expression equals zero, it may be subtracted from the variation in the cost function (52) to give

$$\delta I = \int_{\mathcal{B}} \left[\delta \mathcal{M} - n_i \psi^T \delta \left(F_i - F_{vi}\right)\right] d\mathcal{B}_\xi + \int_{\mathcal{D}} \left[\delta \mathcal{P} + \frac{\partial \psi^T}{\partial \xi_i} \delta \left(F_i - F_{vi}\right)\right] d\mathcal{D}_\xi. \tag{58}$$

Now, since ψ is an arbitrary differentiable function, it may be chosen in such a way that δI no longer depends explicitly on the variation of the state vector δw.

Comparing equations (53) and (55), the variation δw may be eliminated from (58) by equating all field terms with subscript "I" to produce a differential adjoint system governing ψ

$$\frac{\partial \psi^T}{\partial \xi_i} \left[F_{iw} - F_{viw} \right]_I + \mathcal{P}_w = 0 \quad \text{in } \mathcal{D}. \tag{59}$$

The corresponding adjoint boundary condition is produced by equating the subscript "I" boundary terms in equation (58) to produce

$$n_i \psi^T \left[F_{iw} - F_{viw} \right]_I = \mathcal{M}_w \quad \text{on } \mathcal{B}. \tag{60}$$

The remaining terms from equation (58) then yield a simplified expression for the variation of the cost function which defines the gradient

$$\delta I = \int_{\mathcal{B}} \left\{ \delta \mathcal{M}_{II} - n_i \psi^T \left[\delta F_i - \delta F_{vi} \right]_{II} \right\} d\mathcal{B}_\xi + \int_{\mathcal{D}} \left\{ \delta \mathcal{P}_{II} + \frac{\partial \psi^T}{\partial \xi_i} \left[\delta F_i - \delta F_{vi} \right]_{II} \right\} d\mathcal{D}_\xi. \tag{61}$$

Using the relationship between the mesh deformation and the surface modification, the field integral is reduced to a surface integral by integrating along the coordinate lines emanating from the surface. Thus the expression for δI is finally reduced to the form

$$\delta I = \int_{\mathcal{B}} \mathcal{G} \delta \mathcal{F} \, d\mathcal{B}_{\xi}$$

where $\mathcal{F}$ represents the design variables, and $\mathcal{G}$ is the gradient, which is a function defined over the boundary surface.

The boundary conditions satisfied by the flow equations restrict the form of the left hand side of the adjoint boundary condition (60). Consequently, the boundary contribution to the cost function $\mathcal{M}$ cannot be specified arbitrarily. Instead, it must be chosen from the class of functions which allow cancellation of all terms containing δw in the boundary integral of equation (58). On the other hand, there is no such restriction on the specification of the field contribution to the cost function $\mathcal{P}$, since these terms may always be absorbed into the adjoint field equation (59) as source terms.

DERIVATION OF THE VISCOUS ADJOINT TERMS

In computational coordinates, the viscous terms in the Navier–Stokes equations have the form

$$\frac{\partial F_{vi}}{\partial \xi_i} = \frac{\partial}{\partial \xi_i}\left(S_{ij} f_{vj}\right).$$

Computing the variation δw resulting from a shape modification of the boundary, introducing a co-state vector ψ and integrating by parts following the steps outlined by equations (54) to (57) produces

$$\int_{\mathcal{B}} \psi^T \left(\delta S_{2j} f_{vj} + S_{2j} \delta f_{vj}\right) d\mathcal{B}_\xi - \int_{\mathcal{D}} \frac{\partial \psi^T}{\partial \xi_i}\left(\delta S_{ij} f_{vj} + S_{ij} \delta f_{vj}\right) d\mathcal{D}_\xi,$$

where the shape modification is restricted to the coordinate surface $\xi_2 = 0$ so that $n_1 = n_3 = 0$, and $n_2 = 1$.

The viscous terms will be derived under the assumption that the viscosity and heat conduction coefficients μ and k are essentially independent of the flow, and that their variations may be neglected.

TRANSFORMATION TO PRIMITIVE VARIABLES

The derivation of the viscous adjoint terms is simplified by transforming to the primitive variables

$$\tilde{w}^T = (\rho, u_1, u_2, u_3, p)^T,$$

because the viscous stresses depend on the velocity derivatives $\frac{\partial u_i}{\partial x_j}$, while the heat flux can be expressed as

$$\kappa \frac{\partial}{\partial x_i} \left(\frac{p}{\rho} \right).$$

where $\kappa = \frac{k}{R} = \frac{\gamma \mu}{Pr(\gamma - 1)}$.

The relationship between the conservative and primitive variations is defined by the expressions

$$\delta w = M \delta \tilde{w}, \qquad \delta \tilde{w} = M^{-1} \delta w$$

which make use of the transformation matrices $M = \frac{\partial w}{\partial \tilde{w}}$ and $M^{-1} = \frac{\partial \tilde{w}}{\partial w}$.

TRANSFORMATION MATRICES

$$M^T = \begin{bmatrix} 1 & u_1 & u_2 & u_3 & \frac{u_i u_i}{2} \\ 0 & \rho & 0 & 0 & \rho u_1 \\ 0 & 0 & \rho & 0 & \rho u_2 \\ 0 & 0 & 0 & \rho & \rho u_3 \\ 0 & 0 & 0 & 0 & \frac{1}{\gamma - 1} \end{bmatrix}$$

$$M^{-1^T} = \begin{bmatrix} 1 & -\frac{u_1}{\rho} & -\frac{u_2}{\rho} & -\frac{u_3}{\rho} & \frac{(\gamma-1) u_i u_i}{2} \\ 0 & \frac{1}{\rho} & 0 & 0 & -(\gamma - 1) u_1 \\ 0 & 0 & \frac{1}{\rho} & 0 & -(\gamma - 1) u_2 \\ 0 & 0 & 0 & \frac{1}{\rho} & -(\gamma - 1) u_3 \\ 0 & 0 & 0 & 0 & \gamma - 1 \end{bmatrix}$$

CONSERVATIVE AND PRIMITIVE ADJOINT OPERATORS

The conservative and primitive adjoint operators L and $\tilde{L}$ corresponding to the variations δw and $\delta \tilde{w}$ are then related by

$$\int_{\mathcal{D}} \delta w^T L \psi \, d\mathcal{D}_\xi = \int_{\mathcal{D}} \delta \tilde{w}^T \tilde{L} \psi \, d\mathcal{D}_\xi,$$

with

$$\tilde{L} = M^T L,$$

so that after determining the primitive adjoint operator by direct evaluation of the viscous portion of (59), the conservative operator may be obtained by the transformation

$$L = M^{-1^T} \tilde{L}$$

.

CONTRIBUTIONS FROM THE MOMENTUM EQUATIONS

Set $\psi_{j+1} = \phi_j$ for $j = 1, 2, 3$. Then, using the summation convention for repeated indices, the contribution from the momentum equations is

$$\int_{\mathcal{B}} \phi_k \left(\delta S_{2j}\sigma_{kj} + S_{2j}\delta\sigma_{kj}\right) d\mathcal{B}_\xi - \int_{\mathcal{D}} \frac{\partial \phi_k}{\partial \xi_i} \left(\delta S_{ij}\sigma_{kj} + S_{ij}\delta\sigma_{kj}\right) d\mathcal{D}_\xi. \tag{62}$$

The velocity derivatives in the viscous stresses can be expressed as

$$\frac{\partial u_i}{\partial x_j} = \frac{\partial u_i}{\partial \xi_l}\frac{\partial \xi_l}{\partial x_j} = \frac{S_{lj}}{J}\frac{\partial u_i}{\partial \xi_l}$$

with corresponding variations

$$\delta \frac{\partial u_i}{\partial x_j} = \left[\frac{S_{lj}}{J}\right]_I \frac{\partial}{\partial \xi_l}\delta u_i + \left[\frac{\partial u_i}{\partial \xi_l}\right]_{II} \delta\left(\frac{S_{lj}}{J}\right).$$

The variations in the stresses are then

$$\begin{aligned}\delta\sigma_{kj} &= \left\{\mu\left[\frac{S_{lj}}{J}\frac{\partial}{\partial\xi_l}\delta u_k + \frac{S_{lk}}{J}\frac{\partial}{\partial\xi_l}\delta u_j\right] + \lambda\left[\delta_{jk}\frac{S_{lm}}{J}\frac{\partial}{\partial\xi_l}\delta u_m\right]\right\}_I \\ &+ \left\{\mu\left[\delta\left(\frac{S_{lj}}{J}\right)\frac{\partial u_k}{\partial\xi_l} + \delta\left(\frac{S_{lk}}{J}\right)\frac{\partial u_j}{\partial\xi_l}\right] + \lambda\left[\delta_{jk}\delta\left(\frac{S_{lm}}{J}\right)\frac{\partial u_m}{\partial\xi_l}\right]\right\}_{II}.\end{aligned}$$

As before, only those terms with subscript I, which contain variations of the flow variables, need be considered further in deriving the adjoint operator. The field contributions that contain δu_i in equation (62) appear as

$$-\int_{\mathcal{D}}\frac{\partial\phi_k}{\partial\xi_i}S_{ij}\left\{\mu\left(\frac{S_{lj}}{J}\frac{\partial}{\partial\xi_l}\delta u_k + \frac{S_{lk}}{J}\frac{\partial}{\partial\xi_l}\delta u_j\right) + \lambda\delta_{jk}\frac{S_{lm}}{J}\frac{\partial}{\partial\xi_l}\delta u_m\right\}d\mathcal{D}_\xi.$$

This may be integrated by parts to yield

$$\int_{\mathcal{D}}\delta u_k\frac{\partial}{\partial\xi_l}\left(S_{lj}S_{ij}\frac{\mu}{J}\frac{\partial\phi_k}{\partial\xi_i}\right)d\mathcal{D}_\xi + \int_{\mathcal{D}}\delta u_j\frac{\partial}{\partial\xi_l}\left(S_{lk}S_{ij}\frac{\mu}{J}\frac{\partial\phi_k}{\partial\xi_i}\right)d\mathcal{D}_\xi + \int_{\mathcal{D}}\delta u_m\frac{\partial}{\partial\xi_l}\left(S_{lm}S_{ij}\frac{\lambda\delta_{jk}}{J}\frac{\partial\phi_k}{\partial\xi_i}\right)d\mathcal{D}_\xi,$$

where the boundary integral has been eliminated.[2]

[2] By noting that $\delta u_i = 0$ on the solid boundary

By exchanging indices, the field integrals may be combined to produce

$$\int_{\mathcal{D}} \delta u_k \frac{\partial}{\partial \xi_l} S_{lj} \left\{ \mu \left(\frac{S_{ij}}{J} \frac{\partial \phi_k}{\partial \xi_i} + \frac{S_{ik}}{J} \frac{\partial \phi_j}{\partial \xi_i} \right) + \lambda \delta_{jk} \frac{S_{im}}{J} \frac{\partial \phi_m}{\partial \xi_i} \right\} d\mathcal{D}_\xi,$$

which is further simplified by transforming the inner derivatives back to Cartesian coordinates

$$\int_{\mathcal{D}} \delta u_k \frac{\partial}{\partial \xi_l} S_{lj} \left\{ \mu \left(\frac{\partial \phi_k}{\partial x_j} + \frac{\partial \phi_j}{\partial x_k} \right) + \lambda \delta_{jk} \frac{\partial \phi_m}{\partial x_m} \right\} d\mathcal{D}_\xi. \quad (63)$$

The boundary contributions that contain δu_i in equation (62) may be simplified using the fact that

$$\frac{\partial}{\partial \xi_l}\delta u_i = 0 \quad \text{if} \quad l = 1, 3$$

on the boundary $\mathcal{B}$ so that they become

$$\int_{\mathcal{B}} \phi_k S_{2j} \left\{ \mu \left(\frac{S_{2j}}{J} \frac{\partial}{\partial \xi_2} \delta u_k + \frac{S_{2k}}{J} \frac{\partial}{\partial \xi_2} \delta u_j \right) + \lambda \delta_{jk} \frac{S_{2m}}{J} \frac{\partial}{\partial \xi_2} \delta u_m \right\} d\mathcal{B}_\xi. \tag{64}$$

CONTRIBUTIONS FROM THE ENERGY EQUATION

In order to derive the contribution of the energy equation to the viscous adjoint terms it is convenient to set

$$\psi_5 = \theta, \qquad Q_j = u_i\sigma_{ij} + \kappa\frac{\partial}{\partial x_j}\left(\frac{p}{\rho}\right),$$

where the temperature has been written in terms of pressure and density using (49). The contribution from the energy equation can then be written as

$$\int_{\mathcal{B}} \theta\left(\delta S_{2j}Q_j + S_{2j}\delta Q_j\right) d\mathcal{B}_\xi \int_{\mathcal{D}} \frac{\partial\theta}{\partial\xi_i}\left(\delta S_{ij}Q_j + S_{ij}\delta Q_j\right) d\mathcal{D}_\xi. \tag{65}$$

The field contributions that contain δu_i,δp, and $\delta\rho$ in equation (65) appear as

$$-\int_{\mathcal{D}} \frac{\partial\theta}{\partial\xi_i} S_{ij}\delta Q_j d\mathcal{D}_\xi = -\int_{\mathcal{D}} \frac{\partial\theta}{\partial\xi_i} S_{ij}\left\{\delta u_k\sigma_{kj} + u_k\delta\sigma_{kj} + \kappa\frac{S_{lj}}{J}\frac{\partial}{\partial\xi_l}\left(\frac{\delta p}{\rho} - \frac{p}{\rho}\frac{\delta\rho}{\rho}\right)\right\} d\mathcal{D}_\xi. \tag{66}$$

The term involving $\delta\sigma_{kj}$ may be integrated by parts to produce

$$\int_{\mathcal{D}} \delta u_k \frac{\partial}{\partial \xi_l} S_{lj} \left\{ \mu \left(u_k \frac{\partial \theta}{\partial x_j} + u_j \frac{\partial \theta}{\partial x_k} \right) + \lambda \delta_{jk} u_m \frac{\partial \theta}{\partial x_m} \right\} d\mathcal{D}_\xi, \tag{67}$$

where the conditions $u_i = \delta u_i = 0$ are used to eliminate the boundary integral on $\mathcal{B}$. Notice that the other term in (66) that involves δu_k need not be integrated by parts and is merely carried on as

$$-\int_{\mathcal{D}} \delta u_k \sigma_{kj} S_{ij} \frac{\partial \theta}{\partial \xi_i} d\mathcal{D}_\xi \tag{68}$$

The terms in expression (66) that involve δp and $\delta \rho$ may also be integrated by parts to produce both a field and a boundary integral.

The field integral becomes

$$\int_{\mathcal{D}} \left(\frac{\delta p}{\rho} - \frac{p}{\rho} \frac{\delta \rho}{\rho} \right) \frac{\partial}{\partial \xi_l} \left(S_{lj} S_{ij} \frac{\kappa}{J} \frac{\partial \theta}{\partial \xi_i} \right) d\mathcal{D}_\xi$$

which may be simplified by transforming the inner derivative to Cartesian coordinates

$$\int_{\mathcal{D}} \left(\frac{\delta p}{\rho} - \frac{p}{\rho} \frac{\delta \rho}{\rho} \right) \frac{\partial}{\partial \xi_l} \left(S_{lj} \kappa \frac{\partial \theta}{\partial x_j} \right) d\mathcal{D}_\xi. \tag{69}$$

The boundary integral becomes

$$\int_{\mathcal{B}} \kappa \left(\frac{\delta p}{\rho} - \frac{p}{\rho} \frac{\delta \rho}{\rho} \right) \frac{S_{2j} S_{ij}}{J} \frac{\partial \theta}{\partial \xi_i} d\mathcal{B}_\xi. \tag{70}$$

This can be simplified by transforming the inner derivative to Cartesian coordinates

$$\int_{\mathcal{B}} \kappa \left(\frac{\delta p}{\rho} - \frac{p}{\rho} \frac{\delta \rho}{\rho} \right) \frac{S_{2j}}{J} \frac{\partial \theta}{\partial x_j} d\mathcal{B}_\xi, \tag{71}$$

and identifying the normal derivative at the wall

$$\frac{\partial}{\partial n} = S_{2j}\frac{\partial}{\partial x_j}, \tag{72}$$

and the variation in temperature

$$\delta T = \frac{1}{R}\left(\frac{\delta p}{\rho} - \frac{p}{\rho}\frac{\delta \rho}{\rho}\right),$$

to produce the boundary contribution

$$\int_{\mathcal{B}} k\delta T\frac{\partial \theta}{\partial n}d\mathcal{B}_\xi. \tag{73}$$

This term vanishes if T is constant on the wall but persists if the wall is adiabatic.

There is also a boundary contribution left over from the first integration by parts (65) which has the form

$$\int_{\mathcal{B}} \theta\delta\left(S_{2j}Q_j\right) d\mathcal{B}_\xi, \tag{74}$$

where

$$Q_j = k\frac{\partial T}{\partial x_j},$$

since $u_i = 0$. [3]

[3] Notice that for future convenience in discussing the adjoint boundary conditions resulting from the energy equation, both the δw and δS terms corresponding to subscript classes I and II are considered simultaneously.

If the wall is adiabatic

$$\frac{\partial T}{\partial n} = 0,$$

so that using (72),

$$\delta \left(S_{2j} Q_j \right) = 0,$$

and both the δw and δS boundary contributions vanish.

On the other hand, if T is constant $\frac{\partial T}{\partial \xi_l} = 0$ for $l = 1, 3$, so that

$$Q_j = k \frac{\partial T}{\partial x_j} = k \left(\frac{S_l j}{J} \frac{\partial T}{\partial \xi_l} \right) = k \left(\frac{S_{2j}}{J} \frac{\partial T}{\partial \xi_2} \right).$$

Thus, the boundary integral (74) becomes

$$\int_{\mathcal{B}} k\theta \left\{ \frac{{S_{2j}}^2}{J} \frac{\partial}{\partial \xi_2} \delta T + \delta \left(\frac{{S_{2j}}^2}{J} \right) \frac{\partial T}{\partial \xi_2} \right\} d\mathcal{B}_\xi \ . \tag{75}$$

All together, the contributions from the energy equation to the viscous adjoint operator are the three field terms (67), (68) and (69), and either of two boundary contributions (73) or (75), depending on whether the wall is adiabatic or has constant temperature.

THE VISCOUS ADJOINT FIELD OPERATOR

The final form of viscous adjoint operator in primitive variables is

$$
\begin{aligned}
(\tilde{L}\psi)_1 &= -\frac{p}{\rho^2}\frac{\partial}{\partial \xi_l}\left(S_{lj}\kappa\frac{\partial \theta}{\partial x_j}\right) \\
(\tilde{L}\psi)_{i+1} &= \frac{\partial}{\partial \xi_l}\left\{S_{lj}\left[\mu\left(\frac{\partial \phi_i}{\partial x_j}+\frac{\partial \phi_j}{\partial x_i}\right)+\lambda\delta_{ij}\frac{\partial \phi_k}{\partial x_k}\right]\right\} \qquad \text{for} \quad i=1,2,3 \\
&+ \frac{\partial}{\partial \xi_l}\left\{S_{lj}\left[\mu\left(u_i\frac{\partial \theta}{\partial x_j}+u_j\frac{\partial \theta}{\partial x_i}\right)+\lambda\delta_{ij}u_k\frac{\partial \theta}{\partial x_k}\right]\right\}-\sigma_{ij}S_{lj}\frac{\partial \theta}{\partial \xi_l} \\
(\tilde{L}\psi)_5 &= \frac{1}{\rho}\frac{\partial}{\partial \xi_l}\left(S_{lj}\kappa\frac{\partial \theta}{\partial x_j}\right).
\end{aligned}
$$

The conservative viscous adjoint operator may now be obtained by the transformation $L = {M^{-1}}^T \tilde{L}$.

BOUNDARY CONDITIONS ARISING FROM THE MOMENTUM EQUATIONS

The boundary term that arises from the momentum equations including both the δw and δS components (62) takes the form

$$\int_{\mathcal{B}} \phi_k \delta \left(S_{2j} \sigma_{kj} \right) d\mathcal{B}_{\xi}.$$

Replacing the metric term with the corresponding local face area S_2 and unit normal n_j defined by

$$|S_2| = \sqrt{S_{2j} S_{2j}}, \qquad n_j = \frac{S_{2j}}{|S_2|}$$

then leads to

$$\int_{\mathcal{B}} \phi_k \delta \left(|S_2| \, n_j \sigma_{kj} \right) d\mathcal{B}_{\xi}.$$

Defining the components of the surface stress as

$$\tau_k = n_j \sigma_{kj}$$

and the physical surface element

$$dS = |S_2| \, d\mathcal{B}_\xi,$$

the integral may then be split into two components

$$\int_{\mathcal{B}} \phi_k \tau_k \, |\delta S_2| \, d\mathcal{B}_\xi + \int_{\mathcal{B}} \phi_k \delta \tau_k dS, \tag{76}$$

where only the second term contains variations in the flow variables and must consequently cancel the δw terms arising in the cost function. The first term will appear in the expression for the gradient.

A general expression for the cost function that allows cancellation with terms containing $\delta\tau_k$ has the form

$$I = \int_{\mathcal{B}} \mathcal{N}(\tau) dS, \tag{77}$$

corresponding to a variation

$$\delta I = \int_{\mathcal{B}} \frac{\partial \mathcal{N}}{\partial \tau_k} \delta\tau_k dS,$$

for which cancellation is achieved by the adjoint boundary condition

$$\phi_k = \frac{\partial \mathcal{N}}{\partial \tau_k}.$$

Natural choices for $\mathcal{N}$ arise from force optimization and as measures of the deviation of the surface stresses from desired target values.

For viscous force optimization, the cost function should measure friction drag. The friction force in the x_i direction is

$$CD_{fi} = \int_{\mathcal{B}} \sigma_{ij} dS_j = \int_{\mathcal{B}} S_{2j} \sigma_{ij} d\mathcal{B}_\xi$$

so that the force in a direction with cosines q_i has the form

$$C_{qf} = \int_{\mathcal{B}} q_i S_{2j} \sigma_{ij} d\mathcal{B}_\xi.$$

Expressed in terms of the surface stress τ_i, this corresponds to

$$C_{qf} = \int_{\mathcal{B}} q_i \tau_i dS,$$

so that basing the cost function (77) on this quantity gives

$$\mathcal{N} = q_i \tau_i.$$

Cancellation with the flow variation terms in equation (76) therefore mandates the adjoint boundary condition

$$\phi_k = n_k.$$

Note that this choice of boundary condition also eliminates the first term in equation (76) so that it need not be included in the gradient calculation.

In the inverse design case, where the cost function is intended to measure the deviation of the surface stresses from some desired target values, a suitable definition is

$$\mathcal{N}(\tau) = \frac{1}{2} a_{lk} \left(\tau_l - \tau_{dl}\right) \left(\tau_k - \tau_{dk}\right),$$

where τ_d is the desired surface stress, including the contribution of the pressure, and the coefficients a_{lk} define a weighting matrix. For cancellation

$$\phi_k \delta\tau_k = a_{lk} \left(\tau_l - \tau_{dl}\right) \delta\tau_k.$$

This is satisfied by the boundary condition

$$\phi_k = a_{lk} \left(\tau_l - \tau_{dl}\right). \tag{78}$$

Assuming arbitrary variations in $\delta\tau_k$, this condition is also necessary.

In order to control the surface pressure and normal stress one can measure the difference

$$n_j \left\{\sigma_{kj} + \delta_{kj}\left(p - p_d\right)\right\},$$

where p_d is the desired pressure. The normal component is then

$$\tau_n = n_k n_j \sigma_{kj} + p - p_d,$$

so that the measure becomes

$$\begin{aligned}\mathcal{N}(\tau) &= \frac{1}{2}\tau_n^2 \\ &= \frac{1}{2} n_l n_m n_k n_j \left\{\sigma_{lm} + \delta_{lm}\left(p - p_d\right)\right\}\left\{\sigma_{kj} + \delta_{kj}\left(p - p_d\right)\right\}.\end{aligned}$$

This corresponds to setting

$$a_{lk} = n_l n_k$$

in equation (78). Defining the viscous normal stress as

$$\tau_{vn} = n_k n_j \sigma_{kj},$$

the measure can be expanded as

$$\begin{aligned} \mathcal{N}(\tau) &= \frac{1}{2} n_l n_m n_k n_j \sigma_{lm} \sigma_{kj} \\ &+ \frac{1}{2} \left(n_k n_j \sigma_{kj} + n_l n_m \sigma_{lm} \right) (p - p_d) + \frac{1}{2} (p - p_d)^2 \\ &= \frac{1}{2} \tau_{vn}^2 + \tau_{vn} (p - p_d) + \frac{1}{2} (p - p_d)^2 . \end{aligned}$$

For cancellation of the boundary terms

$$\phi_k \left(n_j \delta\sigma_{kj} + n_k \delta p\right) = \left\{n_l n_m \sigma_{lm} + n_l^2 \left(p - p_d\right)\right\} n_k \left(n_j \delta\sigma_{kj} + n_k \delta p\right)$$

leading to the boundary condition

$$\phi_k = n_k \left(\tau_{vn} + p - p_d\right).$$

In the case of high Reynolds number, this is well approximated by the equations

$$\phi_k = n_k \left(p - p_d\right), \tag{79}$$

which should be compared with the single scalar equation derived for the inviscid boundary condition.

BOUNDARY CONDITIONS ARISING FROM THE ENERGY EQUATION

For the adiabatic case, the boundary contribution is (73) while for the constant temperature case the boundary term is (75). One possibility is to introduce a contribution into the cost function which depends on T or $\frac{\partial T}{\partial n}$ so that the appropriate cancellation would occur. Since there is little physical intuition to guide the choice of such a cost function for aerodynamic design, a more natural solution is to set

$$\theta = 0$$

in the constant temperature case or

$$\frac{\partial \theta}{\partial n} = 0$$

in the adiabatic case [4].

[4]Note that in the constant temperature case, this choice of θ on the boundary would also eliminate the boundary metric variation terms in (74)

IMPLEMENTATION OF NAVIER-STOKES DESIGN

The design procedures can be summarized as follows:

1. Solve the flow equations for ρ, u_1, u_2, u_3, p.
2. Solve the adjoint equations for ψ subject to appropriate boundary conditions.
3. Evaluate $\mathcal{G}$.
4. Project $\mathcal{G}$ into an allowable subspace that satisfies any geometric constraints.
5. Update the shape based on the direction of steepest descent.
6. Return to 1 until convergence is reached.

Practical implementation of the viscous design method relies heavily upon fast and accurate solvers for both the state (w) and co-state (ψ) systems.

SEARCH PROCEDURE

The search procedure used in this work is a simple descent method in which small steps are taken in the negative gradient direction.

$$\delta \mathcal{F} = -\lambda \mathcal{G}$$

can be regarded as simulating the time dependent process

$$\frac{d\mathcal{F}}{dt} = -\mathcal{G}$$

where λ is the time step Δt. Let A be the Hessian matrix with element

$$A_{ij} = \frac{\partial \mathcal{G}_i}{\partial \mathcal{F}_j} = \frac{\partial^2 I}{\partial \mathcal{F}_i \partial \mathcal{F}_j}.$$

Suppose that a locally minimum value of the cost function $I^* = I(\mathcal{F}^*)$ is attained when $\mathcal{F} = \mathcal{F}^*$. Then the gradient $\mathcal{G}^* = \mathcal{G}(\mathcal{F}^*)$ must be zero, while the Hessian matrix $A^* = A(\mathcal{F}^*)$ must be positive definite. Since $\mathcal{G}^*$ is zero, the cost function can be expanded as a Taylor series in the neighborhood of $\mathcal{F}^*$ with the form

$$I(\mathcal{F}) = I^* + \frac{1}{2}\left(\mathcal{F} - \mathcal{F}^*\right) A \left(\mathcal{F} - \mathcal{F}^*\right) + \ldots$$

Correspondingly,

$$\mathcal{G}(\mathcal{F}) = A\left(\mathcal{F} - \mathcal{F}^*\right) + \ldots$$

As $\mathcal{F}$ approaches $\mathcal{F}^*$, the leading terms become dominant. Then, setting $\hat{\mathcal{F}} = (\mathcal{F} - \mathcal{F}^*)$, the search process approximates

$$\frac{d\hat{\mathcal{F}}}{dt} = -A^*\hat{\mathcal{F}}.$$

Also, since A^* is positive definite it can be expanded as

$$A^* = RMR^T,$$

where M is a diagonal matrix containing the eigenvalues of A^*, and

$$RR^T = R^T R = I.$$

Setting

$$v = R^T \hat{\mathcal{F}},$$

the search process can be represented as

$$\frac{dv}{dt} = -Mv.$$

The stability region for the simple forward Euler stepping scheme is a unit circle centered at -1 on the negative real axis. Thus for stability we must choose

$$\mu_{\text{max}} \Delta t = \mu_{\text{max}} \lambda < 2,$$

while the asymptotic decay rate, given by the smallest eigenvalue, is proportional to

$$e^{-\mu_{\text{min}} t}.$$

In order to improve the rate of convergence, one can set

$$\delta \mathcal{F} = -\lambda P G,$$

where P is a preconditioner for the search. An ideal choice is $P = A^{*-1}$, so that the corresponding time dependent process reduces to

$$\frac{d\hat{\mathcal{F}}}{dt} = -\hat{\mathcal{F}},$$

for which all the eigenvalues are equal to unity, and $\hat{\mathcal{F}}$ is reduced to zero in one time step by the choice $\Delta t = 1$.

1. Quasi-Newton methods estimate A^* from the change in the gradient during the search process. This requires accurate estimates of the gradient at each time step. In order to obtain these, both the flow solution and the adjoint equation must be fully converged. Most quasi-Newton methods also require a line search in each search direction, for which the flow equations and cost function must be accurately evaluated several times. They have proven quite robust for aerodynamic optimization.
2. An alternative approach which has also proved successful in our previous work is to smooth the gradient and to replace $\mathcal{G}$ by its smoothed value $\bar{\mathcal{G}}$ in the descent process. This both acts as a preconditioner, and ensures that each new shape in the optimization sequence remains smooth.

SMOOTHING THE GRADIENT

Independent movement of the boundary mesh points could produce discontinuities in the designed shape. In order to prevent this the gradient may be smoothed. Suppose that the shape is represented in term of smooth functions such as B-splines, so that

$$\delta \mathcal{F} = Bd,$$

where d is the change of the spline coefficients. Then, using the discrete formulas, to first order the change in the cost is

$$\delta I = \mathcal{G}^T \delta \mathcal{F} = \mathcal{G}^T B d.$$

Thus the gradient with respect to the B-spline coefficients is obtained by multiplying $\mathcal{G}$ by B^T, and a descent step is defined by setting

$$d = -\lambda B^T \mathcal{G}, \;\; \delta \mathcal{F} = Bd = -\lambda B B^T \mathcal{G}$$

where λ is sufficiently small and positive.

IMPLICIT SMOOTHING

Implicit smoothing may also be used. To apply smoothing in the ξ_1 direction, for example, the smoothed gradient $\bar{\mathcal{G}}$ ma be calculated from a discrete approximation to

$$\bar{\mathcal{G}} - \frac{\partial}{\partial \xi_1}\epsilon\frac{\partial}{\partial \xi_1}\bar{\mathcal{G}} = \mathcal{G}$$

where ϵ is the smoothing parameter. If one sets $\delta\mathcal{F} = -\lambda\bar{\mathcal{G}}$, then

$$\begin{aligned}\delta I &= -\iint \mathcal{G}\delta\mathcal{F}\, d\xi_1 d\xi_3 = -\lambda\iint \left(\bar{\mathcal{G}} - \frac{\partial}{\partial \xi_1}\epsilon\frac{\partial\bar{\mathcal{G}}}{\partial \xi_1}\right)\bar{\mathcal{G}}\, d\xi_1 d\xi_3 \\ &= -\lambda\iint \left(\bar{\mathcal{G}}^2 + \epsilon\left(\frac{\partial\bar{\mathcal{G}}}{\partial \xi_1}\right)^2\right) d\xi_1 d\xi_3 < 0,\end{aligned}$$

assuring an improvement if λ is sufficiently small and positive, unless the process has already reached a stationary point at which $\mathcal{G} = 0$.

This results in very large savings in the computational cost.

MODIFIED COST FUNCTION FOR AIRFOIL WITH SHOCKS

In the presence of shock waves the cost function may be modified to the form

$$I = \frac{1}{2}\int\!\!\int \left(\lambda_1 \mathcal{Z} + \lambda_2 \left(\frac{\partial \mathcal{Z}}{\partial \xi_1}\right)^2\right) d\xi_1 d\xi_3 \quad \text{with} \quad \lambda_1 \mathcal{Z} - \frac{\partial}{\partial \xi_1}\lambda_2 \frac{\partial \mathcal{Z}}{\partial \xi_1} = p - p_d.$$

Then

$$\begin{aligned}
\delta I &= \int\!\!\int \left(\lambda_1 \mathcal{Z}\delta\mathcal{Z} + \lambda_2 \frac{\partial \mathcal{Z}}{\partial \xi_1}\frac{\partial}{\partial \xi_1}\delta\mathcal{Z}\right) d\xi_1 d\xi_3 \\
&= \int\!\!\int \mathcal{Z}\left(\lambda_1 - \frac{\partial}{\partial \xi_1}\lambda_2 \frac{\partial}{\partial \xi_1}\right)\delta\mathcal{Z}\, d\xi_1 d\xi_3 \\
&= \int\!\!\int \mathcal{Z}\delta p\, d\xi_1 d\xi_3
\end{aligned}$$

and the smooth quantity $\mathcal{Z}$ replaces $p - p_d$ in the adjoint boundary condition.