AERODYNAMIC SHAPE OPTIMIZATION USING THE ADJOINT METHOD

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☞ THE NAVIER-STOKES EQUATIONS

$$\frac{\partial w}{\partial t} + \frac{\partial f_i}{\partial x_i} = \frac{\partial f_{vi}}{\partial x_i} \quad \text{in } \mathcal{D}, \tag{1}$$

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

$$w = \left\{ \begin{array}{c} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{array} \right\}, \quad f_i = \left\{ \begin{array}{c} \rho u_i \\ \rho u_i u_1 + p\delta_{i1} \\ \rho u_i u_2 + p\delta_{i2} \\ \rho u_i u_3 + p\delta_{i3} \\ \rho u_i H \end{array} \right\}, \quad f_{vi} = \left\{ \begin{array}{c} 0 \\ \sigma_{ij}\delta_{j1} \\ \sigma_{ij}\delta_{j2} \\ \sigma_{ij}\delta_{j3} \\ u_j\sigma_{ij} + k\frac{\partial T}{\partial x_i} \end{array} \right\}. \tag{2}$$

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

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \delta_{ij} \frac{\partial u_k}{\partial x_k}, \tag{3}$$

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

$$k = \frac{c_p \mu}{Pr}, \quad T = \frac{p}{R\rho}. \tag{4}$$

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

$$\frac{\partial\left(Jw\right)}{\partial t} + \frac{\partial\left(F_i - F_{vi}\right)}{\partial \xi_i} = 0 \quad \text{in } \mathcal{D}, \tag{5}$$

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 (5) we have made use of the property that

$$\frac{\partial S_{ij}}{\partial \xi_i} = 0 \ . \tag{6}$$

☞ FORMULATION OF THE OPTIMAL DESIGN PROBLEM FOR THE NAVIER-STOKES EQUATIONS

Suppose that the performance is measured by a cost function

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

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 (5).

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

$$\delta I = \int_{\mathcal{B}} \delta \mathcal{M}(w, S)\, d\mathcal{B}_\xi + \int_{\mathcal{D}} \delta \mathcal{P}(w, S)\, d\mathcal{D}_\xi, \tag{7}$$

with

$$\begin{aligned} \delta \mathcal{M} &= [\mathcal{M}_w]_I\, \delta w + \delta \mathcal{M}_{II}, \\ \delta \mathcal{P} &= [\mathcal{P}_w]_I\, \delta w + \delta \mathcal{P}_{II}, \end{aligned} \tag{8}$$

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 (5) specifies the variation of the state vector δw by

$$\frac{\partial}{\partial \xi_i}\delta\left(F_i - F_{vi}\right) = 0. \tag{9}$$

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

$$\begin{aligned} \delta F_i &= \left[F_{iw}\right]_I \delta w + \delta F_{iII} \\ \delta F_{vi} &= \left[F_{viw}\right]_I \delta w + \delta F_{viII}. \end{aligned} \tag{10}$$

The inviscid contributions are easily evaluated as

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

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

$$\int_{\mathcal{D}} \psi^T \frac{\partial}{\partial \xi_i} \delta \left(F_i - F_{vi} \right) = 0. \tag{11}$$

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

$$\int_{\mathcal{B}} n_i \psi^T \delta \left(F_i - F_{vi} \right) d\mathcal{B}_\xi - \int_{\mathcal{D}} \frac{\partial \psi^T}{\partial \xi_i} \delta \left(F_i - F_{vi} \right) d\mathcal{D}_\xi = 0. \tag{12}$$

Since the left hand expression equals zero, it may be subtracted from the variation in the cost function (7) to give

$$\delta I = \int_{\mathcal{B}} \left[\delta \mathcal{M} - n_i \psi^T \delta \left(F_i - F_{vi} \right) \right] d\mathcal{B}_\xi + \int_{\mathcal{D}} \left[\delta \mathcal{P} + \frac{\partial \psi^T}{\partial \xi_i} \delta \left(F_i - F_{vi} \right) \right] d\mathcal{D}_\xi. \tag{13}$$

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 (8) and (10), the variation δw may be eliminated from (13) by equating all field terms with subscript "I" to produce a differential adjoint system governing ψ

$$\frac{\partial \psi^T}{\partial \xi_i} \left[F_{iw} - F_{viw} \right]_I + \mathcal{P}_w = 0 \quad \text{in } \mathcal{D}. \tag{14}$$

The corresponding adjoint boundary condition is produced by equating the subscript "I" boundary terms in equation (13) to produce

$$n_i \psi^T \left[F_{iw} - F_{viw} \right]_I = \mathcal{M}_w \quad \text{on } \mathcal{B}. \tag{15}$$

The remaining terms from equation (13) then yield a simplified expression for the variation of the cost function which defines the gradient

$$\delta I = \int_{\mathcal{B}} \left\{ \delta \mathcal{M}_{II} - n_i \psi^T \left[\delta F_i - \delta F_{vi} \right]_{II} \right\} d\mathcal{B}_\xi + \int_{\mathcal{D}} \left\{ \delta \mathcal{P}_{II} + \frac{\partial \psi^T}{\partial \xi_i} \left[\delta F_i - \delta F_{vi} \right]_{II} \right\} d\mathcal{D}_\xi \tag{16}$$

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 (15). 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 (13). 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 (14) 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 (9) to (12) 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

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

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 (14), 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

$$\int_{\mathcal{B}} \phi_k \left(\delta S_{2j} \sigma_{kj} + S_{2j} \delta \sigma_{kj} \right) d\mathcal{B}_\xi - \int_{\mathcal{D}} \frac{\partial \phi_k}{\partial \xi_i} \left(\delta S_{ij} \sigma_{kj} + S_{ij} \delta \sigma_{kj} \right) d\mathcal{D}_\xi. \qquad (17)$$

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

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

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 (17) 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.[1]

[1]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

$$\int_{\mathcal{D}} \delta u_k \frac{\partial}{\partial \xi_l} S_{lj} \left\{ \mu \left(\frac{\partial \phi_k}{\partial x_j} + \frac{\partial \phi_j}{\partial x_k} \right) + \lambda \delta_{jk} \frac{\partial \phi_m}{\partial x_m} \right\} d\mathcal{D}_\xi. \tag{18}$$

The boundary contributions that contain δu_i in equation (17) 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

$$\int_{\mathcal{B}} \phi_k S_{2j} \left\{ \mu \left(\frac{S_{2j}}{J}\frac{\partial}{\partial \xi_2}\delta u_k + \frac{S_{2k}}{J}\frac{\partial}{\partial \xi_2}\delta u_j \right) + \lambda \delta_{jk} \frac{S_{2m}}{J}\frac{\partial}{\partial \xi_2}\delta u_m \right\} d\mathcal{B}_\xi. \tag{19}$$

☞ 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

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

where the temperature has been written in terms of pressure and density using (4). The contribution from the energy equation can then be written as

$$\int_{\mathcal{B}} \theta \left(\delta S_{2j} Q_j + S_{2j} \delta Q_j\right) d\mathcal{B}_\xi - \int_{\mathcal{D}} \frac{\partial \theta}{\partial \xi_i} \left(\delta S_{ij} Q_j + S_{ij} \delta Q_j\right) d\mathcal{D}_\xi. \qquad (20)$$

The field contributions that contain δu_i,δp, and $\delta \rho$ in equation (20) appear as

$$-\int_{\mathcal{D}} \frac{\partial \theta}{\partial \xi_i} S_{ij} \delta Q_j d\mathcal{D}_\xi = -\int_{\mathcal{D}} \frac{\partial \theta}{\partial \xi_i} S_{ij} \left\{\delta u_k \sigma_{kj} + u_k \delta \sigma_{kj} + \kappa \frac{S_{lj}}{J} \frac{\partial}{\partial \xi_l}\left(\frac{\delta p}{\rho} - \frac{p}{\rho}\frac{\delta \rho}{\rho}\right)\right\} d\mathcal{D}_\xi. \qquad (21)$$

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

$$\int_{\mathcal{D}} \delta u_k \frac{\partial}{\partial \xi_l} S_{lj} \left\{ \mu \left(u_k \frac{\partial \theta}{\partial x_j} + u_j \frac{\partial \theta}{\partial x_k} \right) + \lambda \delta_{jk} u_m \frac{\partial \theta}{\partial x_m} \right\} d\mathcal{D}_\xi, \tag{22}$$

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 (21) that involves δu_k need not be integrated by parts and is merely carried on as

$$-\int_{\mathcal{D}} \delta u_k \sigma_{kj} S_{ij} \frac{\partial \theta}{\partial \xi_i} d\mathcal{D}_\xi \tag{23}$$

The terms in expression (21) 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

$$\int_{\mathcal{D}} \left(\frac{\delta p}{\rho} - \frac{p}{\rho}\frac{\delta\rho}{\rho} \right) \frac{\partial}{\partial \xi_l} \left(S_{lj} \kappa \frac{\partial \theta}{\partial x_j} \right) d\mathcal{D}_\xi. \tag{24}$$

The boundary integral becomes

$$\int_{\mathcal{B}} \kappa \left(\frac{\delta p}{\rho} - \frac{p}{\rho}\frac{\delta\rho}{\rho} \right) \frac{S_{2j} S_{ij}}{J} \frac{\partial \theta}{\partial \xi_i} d\mathcal{B}_\xi. \tag{25}$$

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

$$\int_{\mathcal{B}} \kappa \left(\frac{\delta p}{\rho} - \frac{p}{\rho}\frac{\delta\rho}{\rho} \right) \frac{S_{2j}}{J} \frac{\partial \theta}{\partial x_j} d\mathcal{B}_\xi, \tag{26}$$

and identifying the normal derivative at the wall

$$\frac{\partial}{\partial n} = S_{2j}\frac{\partial}{\partial x_j}, \tag{27}$$

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

$$\int_{\mathcal{B}} k\delta T \frac{\partial \theta}{\partial n} d\mathcal{B}_{\xi}. \tag{28}$$

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 (20) which has the form

$$\int_{\mathcal{B}} \theta \delta \left(S_{2j} Q_j \right) d\mathcal{B}_\xi, \tag{29}$$

where

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

since $u_i = 0$. [2]

[2] 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 (27),

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

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 (29) becomes

$$\int_{\mathcal{B}} k\theta \left\{ \frac{{S_{2j}}^2}{J} \frac{\partial}{\partial \xi_2} \delta T + \delta \left(\frac{{S_{2j}}^2}{J} \right) \frac{\partial T}{\partial \xi_2} \right\} d\mathcal{B}_\xi \ . \tag{30}$$

All together, the contributions from the energy equation to the viscous adjoint operator are the three field terms (22), (23) and (24), and either of two boundary contributions (28) or (30), 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 (17) takes the form

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

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

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

Defining the components of the surface stress as

$$\tau_k = n_j \left(\delta_{kj} p + \sigma_{kj} \right)$$

and the physical surface element

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

the integral may then be split into two components

$$\int_{\mathcal{B}} \phi_k \tau_k \, |\delta S_2| \, d\mathcal{B}_\xi + \int_{\mathcal{B}} \phi_k \delta \tau_k dS, \tag{31}$$

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

$$I = \int_{\mathcal{B}} \mathcal{N}(\tau) dS, \tag{32}$$

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.

The force in a direction with cosines q_i has the form

$$C_q = \int_{\mathcal{B}} q_i \tau_i dS.$$

If we take this as the cost function (32), this quantity gives

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

Cancellation with the flow variation terms in equation (31) therefore mandates the adjoint boundary condition

$$\phi_k = q_k.$$

Note that this choice of boundary condition also eliminates the first term in equation (31) 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

$$\phi_k = a_{lk} \left(\tau_l - \tau_{dl}\right). \tag{33}$$

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 (33). 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

$$\phi_k = n_k \left(p - p_d\right), \tag{34}$$

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 (28) while for the constant temperature case the boundary term is (30). 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 [3]

[3] Note that in the constant temperature case, this choice of θ on the boundary would also eliminate the boundary metric variation terms in (29).

☞ Design Procedure

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 $\mathcal{G}$ and calculate the corresponding Sobolev gradient $\bar{\mathcal{G}}$.
4. Project $\bar{\mathcal{G}}$ 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.

☞ Design Procedure