AIAA JOURNAL
Vol. 37, No. 1, January 1999

Admitting the Inadmissible: Adjoint Formulation for Incomplete Cost Functionals in Aerodynamic Optimization

Eyal Arian* and Manuel D. Salas†
NASA Langley Research Center, Hampton, Virginia 23681-0001

The adjoint equations are derived for problems in aerodynamic optimization that are improperly considered as inadmissible. For example, a cost functional that depends on the density, rather than on the pressure, is considered inadmissible for an optimization problem governed by the Euler equations. We show that for such problems additional terms should be included in the Lagrangian functional when deriving the adjoint equations. These terms are obtained from the restriction of the interior partial differential equation to the control surface. Demonstrations of the explicit derivation of the adjoint equations for inadmissible cost functionals are given for the potential, Euler, and Navier–Stokes equations.

Nomenclature

A, B	= Jacobian matrices
def	= grad + grad^T
$d\sigma$	= element of integration on the boundary
E	= total specific energy
e	= total energy
H	= enthalpy
I	= unit tensor
k	= coefficient of conductivity
n	= outer normal on the boundary Γ
$\boldsymbol{q}$	= heat conduction vector
R	= local radius of curvature
$\boldsymbol{r}$	= radial unit vector
s	= entropy
T	= temperature
t	= tangential direction on the boundary Γ
$\boldsymbol{U}$	= vector of state variables
$\boldsymbol{u}$	= velocity vector
u_r	= radial component of $\boldsymbol{u}$
u_t	= tangential component of $\boldsymbol{u}$
x, y	= Cartesian coordinates
Γ	= part of the boundary of the domain Ω
γ	= ratio of specific heats
Δ	= Laplace operator
$\boldsymbol{\theta}$	= tangential unit vector
$\boldsymbol{\Lambda}$	= vector of costate variables
$\boldsymbol{\lambda}$	= adjoint velocity vector
$\boldsymbol{\lambda}_r$	= radial component of $\boldsymbol{\lambda}$
$\boldsymbol{\lambda}_t$	= tangential component of $\boldsymbol{\lambda}$
μ	= first viscosity
μ_2	= second viscosity ($\mu_2 + \frac{2}{3}\mu = 0$)
ρ	= density
σ	= stress tensor
τ	= viscous stress tensor
χ	= velocity potential
$\otimes$	= tensor product of two tensors

I. Introduction

IN recent years there has been a growing interest in solving optimization problems governed by the Euler and the Navier–Stokes (N–S) equations (for example, Refs. 1–10). The new interest in this classical field is due to advances in computer performance and improvements in algorithms for the numerical solution of the flow equations. Among the many optimization methods that are being pursued, the Lagrange multiplier method or adjoint method is particularly attractive because of its efficiency for problems with many design variables. The adjoint method is based on a variation analysis of the Lagrangian and requires that the variation vanishes at the optimum. This necessary condition yields an optimality system of coupled partial differential equations (PDEs) consisting of the state equation, the costate or adjoint equation, the optimality condition, and boundary conditions for the state and costate equations.

Recently, Anderson and Venkatakrishnan[8] reported some difficulties in the derivation of boundary conditions for the costate equation for certain cost functionals. The same problem was later reported in Refs. 9 and 10. In Ref. 8, for example, it is concluded that, for aerodynamic optimization problems that are governed by the compressible Euler flow equations, only cost functionals that depend solely on the pressure $F = F(p)$ are admissible, and for viscous flow, using the compressible (N–S) equations, only cost functionals that involve the entire stress tensor, e.g., drag, are admissible. As stated in Ref. 8, the difficulty with the inadmissible cost functionals stems from the need for a suitable balance between the different terms in the variational form of the Lagrangian: For some cost functionals such a balance does not exist, and the requirement that the variation of the Lagrangian vanish does not result in a boundary-value problem for the adjoint variables. In Ref. 9, the authors suggest, for the compressible N–S with adiabatic boundary condition on the solid wall, to introduce a contribution into the cost functional that depends on the temperature so that appropriate cancellation in the variation of the Lagrange functional will occur. In Ref. 10, the authors concluded that no choices of cost functionals, other than those suggested in Ref. 8, lead to a well-posed problem.

From the theory of functional analysis, costate variables exist for all cost functionals.[11] This, however, is not the same as saying that all cost functionals lead to a proper boundary-value problem for the costate equation, which is what we mean by an admissible cost functional.

In this paper, a general method is presented for formulating proper boundary-value problems from cost functionals considered inadmissible in the literature. The method avoids redefining, or introducing new terms in, the cost functional. The term *inadmissible* is obviously incorrect. We claim that for so-called inadmissible cost functionals additional auxiliary boundary equations are needed in the Lagrangian. These relations are obtained from the restriction of the interior PDE and its derivatives (up to the highest order possible) to the boundary. With these additional relations, proper cancellation of terms in the variation of the Lagrange functional can be obtained for any well-defined cost functional. However, there is value in distinguishing those cost functionals that lead to a proper boundary-value problem without the need of auxiliary boundary

Received Feb. 9, 1998; revision received June 29, 1998; accepted for publication Aug. 21, 1998. This paper is declared a work of the U.S. Government and is not subject to copyright protection in the United States.

*Staff Scientist, Institute for Computer Applications in Science and Engineering.
†Director, Institute for Computer Applications in Science and Engineering. Associate Fellow AIAA.

equations from those that do not. To that end, we define complete-cost functionals as those that lead to a well-posed boundary-value problem of the costate equation without need for augmenting the Lagrangian functional with auxiliary boundary equations, and we define incomplete-cost functionals as those requiring the use of auxiliary boundary equations.

The paper is organized as follows: In Sec. II, we begin with the potential equation and an admissible cost functional. This example is intended to illustrate the problem that arises later with the cost functional containing $\partial^2\chi/\partial n^2$, which is also treated in this section. In Sec. III, the adjoint equations are derived for a cost functional containing the density ρ for shape optimization problems governed by the compressible Euler equations. In Sec. IV, the adjoint equations are derived for a cost functional containing only the pressure p for shape optimization problems governed by the compressible N–S equations. In Sec. V, we discuss our findings and make some concluding remarks. Appendix A contains the definition of the Euler Jacobian matrices. Appendix B contains identities of polar coordinates, which are used extensively in Secs. III and IV. Appendix C contains a demonstration of the adjoint derivation on a more complex cost functional than the one presented in Sec. IV for shape optimization problems governed by the compressible N–S equations.

II. Potential Equation

Let Ω be a two-dimensional domain confined in the area between two circles with radii $R_1 < R_2$. We denote by Γ the circle with radius R_1 and by $\partial\Omega - \Gamma$ the circle with radius R_2. Let $f^*(\xi)$ be a given $L^2(\Gamma)$ function defined on the boundary Γ, and let the function $\alpha(\xi)$, defined on Γ, be the design variable.

A. Admissible Cost Functional

Consider first the derivation of the adjoint equation on a Dirichlet cost functional using the standard procedure. The minimization problem is defined as follows:

$$\min_{\alpha} F_1(\chi) = \int_\Gamma (\chi - f^*)^2 \,\mathrm{d}\sigma \tag{1}$$

subject to

$$\begin{aligned} \Delta\,\chi &= 0 \quad \text{in} \quad \Omega \\ \frac{\partial\chi}{\partial n} &= \frac{\partial\alpha}{\partial t} \quad \text{on} \quad \Gamma \\ \chi &= \chi_0 \quad \text{on} \quad \partial\Omega - \Gamma \end{aligned} \tag{2}$$

The definition of the state equation (2) assumes that the design variable α and the state variable χ are smooth enough such that α is differentiable on the boundary and χ is twice differentiable in the interior and that the restriction of its normal derivative to the boundary is well defined. The necessary conditions for a minimum are derived with the adjoint method. We introduce the Lagrange multipliers $\boldsymbol{\lambda}$ defined on the domain Ω, ζ defined on part of the boundary Γ, and ι defined on the rest of the boundary $\partial\Omega - \Gamma$. In terms of the Lagrange multipliers, a Lagrangian is defined by

$$\begin{aligned} \mathcal{L}(\chi, \alpha, \lambda, \zeta, \iota) &= \int_\Gamma (\chi - f^*)^2 \,\mathrm{d}\sigma - \int_\Omega (\lambda\Delta\,\chi)\,\mathrm{d}\Omega \\ &+ \int_\Gamma \zeta\left(\frac{\partial\chi}{\partial n} - \frac{\partial\alpha}{\partial t}\right)\mathrm{d}\sigma + \int_{\partial\Omega-\Gamma} \iota\,(\chi_0 - \chi)\,\mathrm{d}\sigma \end{aligned} \tag{3}$$

The variation of the Lagrangian is given by

$$\begin{aligned} \tilde{\mathcal{L}} &= \int_\Gamma 2\tilde{\chi}(\chi - f^*)\,\mathrm{d}\sigma - \int_\Omega \tilde{\chi}\Delta\,\lambda\,\mathrm{d}\Omega + \int_{\partial\Omega}\left(\tilde{\chi}\frac{\partial\lambda}{\partial n} - \lambda\frac{\partial\tilde{\chi}}{\partial n}\right)\mathrm{d}\sigma \\ &+ \int_\Gamma \zeta\left(\frac{\partial\tilde{\chi}}{\partial n} - \frac{\partial\tilde{\alpha}}{\partial t}\right)\mathrm{d}\sigma + \int_{\partial\Omega-\Gamma} \iota\,\tilde{\chi}\,\mathrm{d}\sigma \end{aligned} \tag{4a}$$

$$\begin{aligned} \tilde{\mathcal{L}} &= -\int_\Omega \tilde{\chi}\Delta\,\lambda\,\mathrm{d}\Omega + \int_\Gamma \tilde{\chi}\left[\frac{\partial\lambda}{\partial n} + 2(\chi - f^*)\right]\mathrm{d}\sigma \\ &+ \int_\Gamma \frac{\partial\tilde{\chi}}{\partial n}(\zeta - \lambda)\,\mathrm{d}\sigma + \int_{\partial\Omega-\Gamma} \frac{\partial\tilde{\chi}}{\partial n}\lambda\,\mathrm{d}\sigma + \int_\Gamma \tilde{\alpha}\frac{\partial\zeta}{\partial t}\,\mathrm{d}\sigma \end{aligned} \tag{4b}$$

The term containing $\tilde{\chi}$ on $\partial\Omega - \Gamma$ was omitted because χ is fixed on that part of the boundary [see Eq. (2)], and therefore, its variation vanishes.

The necessary conditions for a minimum are obtained by requiring that the integrands in Eq. (4b) vanish. Matching the terms that multiply $\tilde{\chi}$ and those that multiply $\partial\tilde{\chi}/\partial n$ results in the following equations:

$$\begin{aligned} &\tilde{\chi}(\Omega): && \Delta\,\lambda = 0 && \text{in} && \Omega \\ &\tilde{\chi}(\Gamma): && \frac{\partial\lambda}{\partial n} = -2(\chi - f^*) && \text{on} && \Gamma \\ &\frac{\partial\tilde{\chi}}{\partial n}(\Gamma): && \zeta = \lambda && \text{on} && \Gamma \\ &\frac{\partial\tilde{\chi}}{\partial n}(\partial\Omega - \Gamma): && \lambda = 0 && \text{on} && \partial\Omega - \Gamma \\ &\tilde{\alpha}(\Gamma): && \frac{\partial\zeta}{\partial t} = 0 && \text{on} && \Gamma \end{aligned}$$

Therefore, the costate (adjoint) boundary-value problem is defined by

$$\begin{aligned} \Delta\,\lambda &= 0 \quad \text{in} \quad \Omega \\ \frac{\partial\lambda}{\partial n} &= -2(\chi - f^*) \quad \text{on} \quad \Gamma \\ \lambda &= 0 \quad \text{on} \quad \partial\Omega - \Gamma \end{aligned} \tag{5}$$

with the Fréchet derivative of the cost functional with respect to α given by

$$\frac{\mathrm{d}F_1}{\mathrm{d}\alpha} = \frac{\partial\lambda}{\partial t} \quad \text{on} \quad \Gamma \tag{6}$$

B. Inadmissible Cost Functional

Suppose that we want to minimize a cost functional that depends on the second normal derivative on the boundary. Then the minimization problem is defined as follows:

$$\min_{\alpha} F_2(\chi) = \int_\Gamma \left(\frac{\partial^2\chi}{\partial n^2} - f^*\right)^2 \mathrm{d}\sigma \tag{7}$$

subject to Eq. (2). However, the definition of the cost functional (7) assumes that the second normal derivative of χ on the boundary exists and is in $L^2(\Gamma)$. This is not consistent with the smoothness requirement of χ at Sec. II.A unless we additionally assume that α is smoother than required by the state PDE, i.e., that α is twice differentiable on the boundary and that the restriction of its second normal derivative to the boundary is well defined. If we derive the necessary conditions for a minimum as we did for the Dirichlet cost functional (1), then the variation of the Lagrangian is given by

$$\begin{aligned} \tilde{\mathcal{L}} &= \int_\Gamma 2\frac{\partial^2\tilde{\chi}}{\partial n^2}\left(\frac{\partial^2\chi}{\partial n^2} - f^*\right)\mathrm{d}\sigma - \int_\Omega (\tilde{\chi}\Delta\,\lambda)\,\mathrm{d}\Omega \\ &+ \int_{\partial\Omega}\left(\tilde{\chi}\frac{\partial\lambda}{\partial n} - \lambda\frac{\partial\tilde{\chi}}{\partial n}\right)\mathrm{d}\sigma + \int_\Gamma \zeta\left(\frac{\partial\tilde{\chi}}{\partial n} - \frac{\partial\tilde{\alpha}}{\partial t}\right)\mathrm{d}\sigma \end{aligned} \tag{8}$$

(As earlier discussed, the term that contains $\tilde{\chi}$ on the far field, $\partial\Omega - \Gamma$, was omitted.)

In the preceding example, we saw how the first and third terms in the variation of the Lagrangian (4a) combined to give a boundary condition for $\partial\lambda/\partial n$ along Γ. In this example, the first term in Eq. (8), the term with $\partial^2\tilde{\chi}/\partial n^2$, cannot be combined with any of the other terms on the boundary Γ and, hence, we cannot obtain a boundary condition on Γ for the costate equation. A cost functional exhibiting this behavior was termed inadmissible in the literature.[8] However, because the state equation (2) is linear, χ depends on α linearly, and the cost functional F_2 is a quadratic in α. A quadratic cost functional has a unique minimizer; thus, the cost functional F_2 is, in fact, admissible.

Next we show how to overcome this problem using an auxiliary boundary equation.

C. Auxiliary Boundary Equation

For convenience, let us introduce polar coordinates (r, θ). In polar coordinates, the restriction of the interior PDE (2) to the boundary

Γ results in the following auxiliary boundary equation (ABE) (assuming that the solution is smooth enough):

$$\frac{1}{R_1}\frac{\partial \chi}{\partial r} + \frac{\partial^2 \chi}{\partial r^2} + \frac{1}{R_1^2}\frac{\partial^2 \chi}{\partial \theta^2} = 0 \qquad \text{on} \qquad \Gamma \tag{9}$$

Here we assume that $\hat{r} = -\hat{n}$ is perpendicular to the boundary, pointing into the domain, and R_1 is the radius of curvature. By Eq. (9) we get ($\mathrm{d}t = R_1\,\mathrm{d}\theta$)

$$\frac{\partial^2 \tilde{\chi}}{\partial r^2} = \left(-\frac{1}{R_1}\frac{\partial \tilde{\chi}}{\partial r} - \frac{\partial^2 \tilde{\chi}}{\partial t^2}\right) \qquad \text{on} \qquad \Gamma \tag{10}$$

which can be used to replace $\partial^2\tilde{\chi}/\partial n^2$ in the variation of the Lagrangian. Integration by parts, along the boundary, of the term containing tangential derivatives results in a variational form of the Lagrangian that contains only the naturally occurring boundary terms ($\tilde{\chi}$ and $\partial\tilde{\chi}/\partial r$).

Another way to use Eq. (9), which leads to the same result, is by adding it to the Lagrangian with a new Lagrange multiplier η. Then $\tilde{\mathcal{L}}$ is augmented with the term

$$\int_\Gamma \eta\left(-\frac{1}{R_1}\frac{\partial \tilde{\chi}}{\partial r} - \frac{\partial^2 \tilde{\chi}}{\partial r^2} - \frac{\partial^2 \tilde{\chi}}{\partial t^2}\right)\mathrm{d}\sigma$$

which results in the following adjoint equations on the boundary:

$$\begin{aligned} \frac{\partial^2 \tilde{\chi}}{\partial r^2}(\Gamma)&: \qquad -\eta + 2\left(\frac{\partial^2 \chi}{\partial r^2} - f^*\right) = 0 \\ \tilde{\chi}(\Gamma)&: \qquad -\frac{\partial^2 \eta}{\partial t^2} - \frac{\partial \lambda}{\partial r} = 0 \\ -\frac{\partial \tilde{\chi}}{\partial r}(\Gamma)&: \qquad \frac{1}{R_1}\eta - \lambda + \zeta = 0 \end{aligned} \tag{11}$$

Therefore, the adjoint equations can be written in the following strong form:

$$\begin{aligned} \Delta\lambda &= 0 \qquad \text{in} \qquad \Omega \\ -\frac{\partial \lambda}{\partial r} &= 2\left(\frac{\partial^4 \chi}{\partial r^2 \partial t^2} - \frac{\partial^2 f^*}{\partial t^2}\right) \qquad \text{on} \qquad \Gamma \\ \lambda &= 0 \qquad \text{on} \qquad \partial\Omega - \Gamma \end{aligned} \tag{12}$$

The Fréchet derivative of the cost functional F_2 with respect to α is then given by

$$\frac{\mathrm{d}F_2}{\mathrm{d}\alpha} = \frac{\partial \zeta}{\partial t} = \frac{\partial \lambda}{\partial t} - \frac{2}{R_1}\left(\frac{\partial^3 \chi}{\partial r^2 \partial t} - \frac{\partial f^*}{\partial t}\right) \qquad \text{on} \qquad \Gamma \tag{13}$$

In the same manner, other cost functionals can be treated by taking (if necessary and consistent with the smoothness assumption of the cost functional definition) higher derivatives of $\Delta\chi = 0$, restricting the resulting equations to the boundary and adding them to the Lagrangian with additional Lagrange multipliers.

We add a remark on the required smoothness of the Lagrange multipliers. If we insist on solving the adjoint equation in its strong form (12), then the smoothness requirement of the state solution should be even stronger than assumed in Sec. II.B. [Also $f^*(s)$ should be smoother than $L^2(\Gamma)$.] This requirement can be relaxed if the adjoint equations are solved in a weak formulation, for example, by finite elements.[11] For future reference we give the following definition:

Definition. We define a complete-cost functional as one that leads to a boundary-value problem of the costate equation without the need for augmenting the Lagrangian functional with ABEs. Otherwise, the cost functional will be termed as incomplete.

In the next sections we treat similarly higher-level models of fluid dynamics PDE. In these cases, the functional analysis of the smoothness properties of the state equations are not as obvious as in the preceding example.

III. Euler Equations

For simplicity, the derivation is done in two dimensions. Let $\boldsymbol{U}$ denote the vector of state variables:

$$\boldsymbol{U} = (\rho, \rho u, \rho v, \rho E)^T \tag{14}$$

The Euler equations are given by (conservative form)

$$\begin{aligned} \mathrm{div}(\rho\boldsymbol{u}) = 0, \qquad \mathrm{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u} + pI) = 0 \\ \mathrm{div}(\rho\boldsymbol{u}H) = 0 \end{aligned} \tag{15}$$

where $\boldsymbol{u}\cdot\boldsymbol{n} = 0$ on the solid wall Γ and with additional appropriate boundary conditions on the far field. [The preceding system, in the interior, can be written in an equivalent form in terms of the Jacobian matrices; $\nabla(\boldsymbol{A}\boldsymbol{U}) = 0$, where the Jacobian matrices $\boldsymbol{A} = (A, B)$ are given in Appendix A.]

The following are state relations for the pressure p and the total enthalpy H:

$$\begin{aligned} p &= (\gamma - 1)\rho E - [(\gamma - 1)/2]\rho|\boldsymbol{u}|^2 \\ H &= [\gamma/(\gamma - 1)](p/\rho) + (|\boldsymbol{u}|^2/2) \end{aligned} \tag{16}$$

A. Natural Boundary Terms

Integrating by parts, the Euler equations results in a term containing the pressure on the boundary:

$$\int_\Omega \nabla(\boldsymbol{A}\boldsymbol{U})\,\mathrm{d}\Omega = \int_{\partial\Omega} p(0, n_1, n_2, 0)^T\,\mathrm{d}\sigma \tag{17}$$

(in polar coordinates $n_1 = -1$ and $n_2 = 0$); therefore, any minimization problem that contains terms other than the pressure will result in noncanceling terms in the variational Lagrangian.

B. Example of an Incomplete Cost Functional

The following cost functional is incomplete (the design variable is the shape of the solid wall Γ):

$$F(\rho) = \int_\Gamma (\rho - \rho^*)^2\,\mathrm{d}\sigma \tag{18}$$

The Lagrangian is given by

$$\mathcal{L} = \int_\Gamma (\rho - \rho^*)^2\,\mathrm{d}\sigma + \int_\Omega \boldsymbol{\Lambda}^T\nabla(\boldsymbol{A}\boldsymbol{U})\,\mathrm{d}\Omega + \int_\Gamma \zeta(\boldsymbol{u}\cdot\boldsymbol{n})\,\mathrm{d}\sigma + \text{far-field terms} \tag{19}$$

where $\boldsymbol{\Lambda}$ is the vector of costate variables,

$$\boldsymbol{\Lambda} = (\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \boldsymbol{\lambda}_3, \boldsymbol{\lambda}_4)^T \tag{20}$$

and we denote by $\boldsymbol{\lambda}$ the adjoint velocity vector, i.e.,

$$\boldsymbol{\lambda} = (\boldsymbol{\lambda}_2, \boldsymbol{\lambda}_3) \tag{21}$$

The variation of the Lagrangian is given by

$$\tilde{\mathcal{L}} = \int_\Gamma 2\tilde{\rho}(\rho - \rho^*)\,\mathrm{d}\sigma + \int_\Omega \tilde{\boldsymbol{U}}\left(A^T\boldsymbol{\Lambda}_x + B^T\boldsymbol{\Lambda}_y\right)\mathrm{d}\Omega + \int_\Gamma \tilde{p}\boldsymbol{\lambda}_2\,\mathrm{d}\sigma + \int_\Gamma \tilde{\alpha}g(\boldsymbol{U}, \boldsymbol{\Lambda})\,\mathrm{d}\sigma + \text{far-field terms} \tag{22}$$

which results in noncancellation of terms in $\tilde{\mathcal{L}}$ because the cost functional is not given in terms of the natural boundary term p. [In fact, for shape optimization problems, as we discuss here, the variation of the Lagrangian includes more terms on the boundary Γ that depend on $\tilde{\boldsymbol{u}}\cdot\boldsymbol{n}$. However, these terms contribute only to the gradient term

$$\int_\Gamma \tilde{\alpha}g(\boldsymbol{U}, \boldsymbol{\Lambda})\,\mathrm{d}\sigma$$

and, therefore, do not play a role in the derivation of the adjoint boundary-value problem. For simplicity we do not discuss these terms in this paper.]

However, in general, we can write

$$\rho = \rho(p, s) \tag{23}$$

where s is the entropy, and, in particular, on the surface Γ we can write

$$\rho = \rho(p) \tag{24}$$

in the absence of shock waves because the entropy is constant along the streamline wetting the surface. [In the presence of shocks, it is still valid to write $\rho = \rho(p)$ in a piecewise sense between shocks using the Rankine–Hugoniot conditions to connect the piecewise regions along the streamline wetting the surface.] Hence, we know that we can overcome this problem. In the next section we derive the adjoint equations for the incomplete cost functional (18), with a general procedure, along the lines of Sec. II.C.

C. ABEs

As in the potential problem we derive ABEs by restricting the interior PDEs to the boundary. For simplicity, we examine the resulting equation locally around a point on the boundary and use polar coordinates. Figure 1 shows the local coordinate system. Throughout we use the unit tangential vector $\boldsymbol{t}$ on the boundary instead of $\boldsymbol{\theta}$. Note that on the boundary Γ

$$\frac{\partial}{\partial t} = \frac{1}{R}\frac{\partial}{\partial \boldsymbol{\theta}} \tag{25}$$

Also, in polar coordinates the components of the velocity vector $\boldsymbol{u}$ will be denoted by $\boldsymbol{u} = (u_r, u_t)$, where $u_r = \boldsymbol{u}\cdot\boldsymbol{r}$ and $u_t = \boldsymbol{u}\cdot\boldsymbol{\theta}$; similarly, the components of the adjoint velocity vector $\boldsymbol{\lambda}$ will be denoted by $\boldsymbol{\lambda} = (\boldsymbol{\lambda}_r, \boldsymbol{\lambda}_t)$, where $\boldsymbol{\lambda}_r = \boldsymbol{\lambda}\cdot\boldsymbol{r}$ and $\boldsymbol{\lambda}_t = \boldsymbol{\lambda}\cdot\boldsymbol{\theta}$.

Continuity Equation

In polar coordinates, on the boundary, the continuity equation is given by $[\nabla(\rho\boldsymbol{u}) = 0]$

$$\frac{\partial}{\partial r}(\rho u_r) + \frac{\partial}{\partial t}(\rho u_t) = 0 \tag{26}$$

Also, higher-order derivatives of the continuity equation can be taken and restricted to the boundary and are considered auxiliary boundary equations as long as the solution in the interior is smooth enough so that these derivatives exist.

Momentum Equations

The momentum equations, $\nabla\cdot(\rho\boldsymbol{u}\otimes\boldsymbol{u} + pI) = 0$, in polar coordinates are given by [see Eq. (B4)]

$$\begin{aligned} &\frac{\partial}{\partial r}\left(\rho u_r^2\right) + \frac{\rho u_r^2}{r} + \frac{1}{r}\frac{\partial}{\partial\theta}(\rho u_r u_t) - \frac{\rho u_t^2}{r} + \frac{\partial p}{\partial r} = 0 \\ &\frac{\partial}{\partial r}(\rho u_r u_t) + 2\frac{\rho u_r u_t}{r} + \frac{1}{r}\frac{\partial}{\partial\theta}\left(\rho u_t^2\right) + \frac{\partial p}{\partial t} = 0 \end{aligned} \tag{27}$$

Using the solid wall boundary condition and relation (26), the restriction of Eq. (27) to the boundary results in

$$-\frac{\rho u_t^2}{R} + \frac{\partial p}{\partial r} = 0, \qquad \rho u_t\frac{\partial u_t}{\partial t} + \frac{\partial p}{\partial t} = 0 \tag{28}$$

where R is the local radius of curvature (Fig. 1).

Higher-order equations can be derived by taking derivatives of Eqs. (27) and restricting them to the boundary.

Energy Equation

The energy equation in polar coordinates is given by $[\nabla\cdot(\rho\boldsymbol{u}H) = 0]$

$$\frac{1}{r}\frac{\partial}{\partial\theta}(\rho u_t H) + \frac{1}{r}\frac{\partial}{\partial r}(\rho r u_r H) = 0 \tag{29}$$

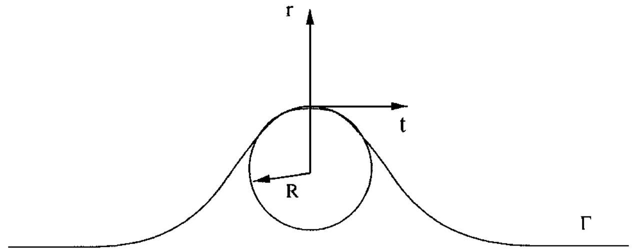

Fig. 1 Local coordinate system around a point on the boundary.

Using the solid wall boundary condition and relation (26), the restriction of Eq. (29) to the boundary results in

$$\frac{\partial H}{\partial t} = 0 \qquad \text{or} \qquad H = \text{const on } \Gamma \tag{30}$$

Derivation of the Adjoint Equations

The definition of the cost functional (18) contains an implicit assumption that the restriction of the density state variable to the solid wall is continuous [and also that $\rho(\Gamma)\in L^2(\Gamma)$]. However, in general, the density is not continuous in the direction perpendicular to streamlines, whereas the pressure p and the normal velocity u_r are always continuous in that direction.[12] The new assumption on the smoothness of the density is introduced into the Lagrangian by adding the ABEs:

$$\begin{aligned} \mathcal{L}_{\text{ABE}} = \int_\Gamma \Bigg\{ &\eta_1\left[\frac{\partial}{\partial n}(\rho\boldsymbol{u}\cdot\boldsymbol{n}) + \frac{\partial}{\partial t}(\rho\boldsymbol{u}\cdot\boldsymbol{t})\right] \\ &+ \eta_2\left(-\frac{\rho u_2^2}{r} + \frac{\partial p}{\partial r}\right) + \eta_3\left(\rho u_t\frac{\partial u_t}{\partial t} + \frac{\partial p}{\partial t}\right) + \eta_4 H\Bigg\}\,\mathrm{d}\sigma \end{aligned} \tag{31}$$

where $(\eta_1,\ldots,\eta_4)$ are additional Lagrange multipliers. For the cost functional (18), the restriction of the continuity and first momentum equations are not required, and therefore, we choose $\eta_1 = \eta_2 = 0$. The variation of the enlarged Lagrangian, $\mathcal{L} + \mathcal{L}_{\text{ABE}}$, yields three adjoint equations on the boundary for $\boldsymbol{\lambda}$, η_3, and η_4:

$$\begin{aligned} &\tilde{\rho}(\Gamma): && \eta_3 u_t\frac{\partial u_t}{\partial t} - \eta_4\frac{\gamma}{\gamma-1}\frac{p}{\rho^2} + 2(\rho-\rho^*) = 0 \\ &\tilde{u}_t(\Gamma): && \eta_3\rho\frac{\partial u_t}{\partial t} - \frac{\partial}{\partial t}(\rho u_t\eta_3) + \eta_4 u_t = 0 \\ &\tilde{p}(\Gamma): && -\frac{\partial\eta_3}{\partial t} + \frac{\gamma}{\gamma-1}\eta_4\frac{1}{\rho} + \boldsymbol{\lambda}_r = 0 \end{aligned} \tag{32}$$

where we have used the relation

$$\tilde{H} = [\gamma/(\gamma-1)][(\tilde{p}/\rho) - (p/\rho^2)\tilde{\rho}] + u_t\tilde{u}_t = 0 \tag{33}$$

[We assume that the term defined on the endpoints of Γ, which results from the integration by parts

$$\int_\Gamma \eta_3\frac{\partial p}{\partial t}\,\mathrm{d}\sigma$$

is equal to zero, i.e., $\eta_3 p(\partial\Gamma^+) - \eta_3 p(\partial\Gamma^-) = 0$.] System (32) can be solved by solving the first two PDEs in Eq. (32) for η_3 and η_4 and substituting the result in the third equation, which is the transpiration boundary condition for $\boldsymbol{\lambda}$.

IV. N–S Equations

The compressible N–S equations are given by

$$\begin{aligned} &\operatorname{div}(\rho\boldsymbol{u}) = 0, \qquad \operatorname{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u}) = \operatorname{div}(\sigma) \\ &\operatorname{div}(e\boldsymbol{u}) + \operatorname{div}(\boldsymbol{q}) = \operatorname{div}(\sigma\boldsymbol{u}) \end{aligned} \tag{34}$$

where the stress tensor σ is given by

$$\sigma = -pI + \mu_2\operatorname{div}(\boldsymbol{u})I + \mu\operatorname{def}(\boldsymbol{u})$$

The heat conduction vector is related to the temperature and the coefficient of conductivity (set equal to a constant) by the relation $\boldsymbol{q} = -k\,\mathrm{grad}(T)$. The total energy satisfies $e = \rho(|\boldsymbol{u}|^2/2) + \rho[T/\gamma(\gamma-1)]$.

The solid wall boundary conditions are given by

$$\boldsymbol{u} = 0, \qquad aT + b\frac{\partial T}{\partial n} = c \tag{35}$$

where a, b, and c are parameters. (We set $a = c = 0$ and $b = 1$, resulting in the adiabatic wall boundary condition.)

A. Natural Boundary Terms

For simplicity we will denote the system of N–S equations by $\nabla \cdot \boldsymbol{F} = 0$, where $\boldsymbol{F}$ consists of the flux vectors. Integration by parts of the compressible N–S equations results in the following boundary terms:

$$\int_\Omega (\nabla \cdot \boldsymbol{F})\,\mathrm{d}\Omega = \int_{\partial\Omega} (0, (\sigma\boldsymbol{n})_1, (\sigma\boldsymbol{n})_2, 0)^T\,\mathrm{d}\sigma \tag{36}$$

Therefore, the natural boundary terms for the compressible N–S equations are the total fluid force components $(\sigma\boldsymbol{n})_j$. (In other words, the only complete cost functionals are those that measure lift or drag.)

B. Example of an Incomplete Cost Functional

Let us take, for example, the following cost functional, which is incomplete (here, as in the preceding section, the design variable is the shape Γ) because its variation is not given in terms of the force components in Eq. (36):

$$F(p) = \int_\Gamma (p - p^*)^2\,\mathrm{d}\sigma \tag{37}$$

The cost functional (37) was treated in Ref. 13 by neglecting a term in the Lagrangian and in Ref. 8 by modifying the cost functional. A demonstration of the adjoint derivation on a more complex cost functional is given in Appendix C.

The Lagrangian is given by

$$\mathcal{L} = \int_\Gamma (p-p^*)^2\,\mathrm{d}\sigma + \int_\Omega \boldsymbol{\Lambda}^T \cdot (\nabla\cdot\boldsymbol{F})\,\mathrm{d}\Omega + \int_\Gamma \zeta\frac{\partial T}{\partial n}\,\mathrm{d}\sigma + \int_\Gamma \iota\cdot\boldsymbol{u}\,\mathrm{d}\sigma + \text{far-field terms} \tag{38}$$

The variation of the Lagrangian is given by

$$\tilde{\mathcal{L}} = \text{interior terms} + \int_\Gamma 2\tilde{p}(p-p^*)\,\mathrm{d}\sigma + \int_{\partial\Omega}\left[-\tilde{T}k\frac{\partial\lambda_4}{\partial r} + \frac{\partial\tilde{T}}{\partial r}k\lambda_4 + \frac{\partial\tilde{u}_r}{\partial r}\frac{4}{3}\mu\lambda_r + \frac{\partial\tilde{u}_t}{\partial r}\mu\lambda_t + \tilde{p}\lambda_r\right]\mathrm{d}\sigma + \int_\Gamma \tilde{\alpha}g(\boldsymbol{U},\boldsymbol{\Lambda})\,\mathrm{d}\sigma \tag{39}$$

The term $\partial\tilde{T}/\partial r$ does not contribute to the adjoint equations (assuming adiabatic boundary conditions) and, therefore, will be omitted. (By the same reasoning the term containing the variation of $\boldsymbol{u}$ on Γ and the variation of the far-field terms vanish.) Also note that the variation in T can be transformed to variations in p and ρ using the equation of state $T = p/(\gamma-1)\rho$. The cost functional (37) is considered incomplete because the term $\partial\tilde{u}_r/\partial r$ determines the adjoint boundary condition $\boldsymbol{\lambda}_r = 0$. As a result, we do not obtain a boundary-value problem representation of the adjoint equations.

C. ABEs

Continuity Equation

Because the boundary condition on Γ implies that $(\partial/\partial t)(\rho u_t) = 0$, we get from the continuity equation that [see Eq. (26)]

$$\frac{\partial u_r}{\partial r} = 0 \tag{40}$$

Momentum Equations

Let us write the momentum equations in the form

$$\mathrm{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u}) = \mathrm{div}(\sigma) = \mathrm{div}(-pI) + \mathrm{div}(\tau)$$

The term $\mathrm{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u} + pI)$ is given in polar coordinates in Eq. (27). Taking the limit to the boundary, we get that

$$\lim_{x\to\Gamma}\mathrm{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u}) = 0$$

The term τ in polar coordinates is given by

$$\tau = \mu_2\,\mathrm{div}(\boldsymbol{u})I + \mu\,\mathrm{def}(\boldsymbol{u}) = \begin{bmatrix} \mu_2\,\mathrm{div}(\boldsymbol{u}) + 2\mu\dfrac{\partial u_r}{\partial r} & \mu\left(\dfrac{\partial u_r}{\partial t} - \dfrac{u_t}{r} + \dfrac{\partial u_t}{\partial r}\right) \\ \mu\left(\dfrac{\partial u_r}{\partial t} - \dfrac{u_t}{r} + \dfrac{\partial u_t}{\partial r}\right) & \mu_2\,\mathrm{div}(\boldsymbol{u}) + 2\mu\left(\dfrac{\partial u_t}{\partial t} + \dfrac{u_r}{r}\right) \end{bmatrix}$$

Evaluating $\mathrm{div}(\tau)$ on the boundary and using the identities

$$\lim_{x\to\Gamma}\mathrm{div}(\boldsymbol{u}) = 0, \qquad \lim_{x\to\Gamma}\frac{\partial}{\partial r}\mathrm{div}(\boldsymbol{u}) = -\frac{1}{\rho}\frac{\partial\rho}{\partial t}\frac{\partial u_t}{\partial r} \tag{41}$$

results in the following auxiliary momentum boundary equations [see Eq. (B4)]:

$$\begin{gathered}\frac{\partial p}{\partial r} + \mu_2\frac{1}{\rho}\frac{\partial\rho}{\partial t}\frac{\partial u_t}{\partial r} - 2\mu\frac{\partial^2 u_r}{\partial r^2} - \mu\frac{\partial^2 u_t}{\partial r\partial t} = 0 \\ \frac{\partial p}{\partial t} - \mu\frac{\partial^2 u_t}{\partial r^2} - \frac{1}{R}\mu\frac{\partial u_t}{\partial r} = 0\end{gathered} \tag{42}$$

Energy Equation

The energy equation is given by

$$\mathrm{div}(e\boldsymbol{u}) + \mathrm{div}(\boldsymbol{q}) = \mathrm{div}(\sigma\boldsymbol{u})$$

Using the relation

$$e\boldsymbol{u} = \left[\rho\frac{|\mathbf{u}|^2}{2} + \frac{\rho}{\gamma(\gamma-1)}T\right]\boldsymbol{u}$$

and taking its divergence in polar coordinates, we get

$$\lim_{x\to\Gamma}\mathrm{div}(e\boldsymbol{u}) = 0 \tag{43}$$

The term $\mathrm{div}(\boldsymbol{q}) = -k\Delta T$ satisfies (assuming an adiabatic boundary condition)

$$\lim_{x\to\Gamma}\mathrm{div}(\boldsymbol{q}) = -k\left(\frac{\partial^2 T}{\partial r^2} + \frac{\partial^2 T}{\partial t^2}\right) \tag{44}$$

The term $\sigma\boldsymbol{u}$ and its tangential derivatives on the boundary are zero; therefore, only its radial derivative is considered:

$$\lim_{x\to\Gamma}\mathrm{div}(\sigma\boldsymbol{u}) = \mu\left(\frac{\partial u_t}{\partial r}\right)^2 \tag{45}$$

Equations (43–45) imply the following auxiliary energy boundary equation:

$$-k\left(\frac{\partial^2 T}{\partial r^2} + \frac{\partial^2 T}{\partial t^2}\right) - \mu\left(\frac{\partial u_t}{\partial r}\right)^2 = 0 \tag{46}$$

Derivation of the Adjoint Equations

As in the Euler case, we add the ABEs to the Lagrangian:

$$\mathcal{L}_{\mathrm{ABE}} = \int_\Gamma\left\{\eta_1\left(\frac{\partial u_r}{\partial r}\right) + \eta_2\left(\frac{\partial p}{\partial r} + \mu_2\frac{1}{\rho}\frac{\partial\rho}{\partial t}\frac{\partial u_t}{\partial r} - 2\mu\frac{\partial^2 u_r}{\partial r^2} - \mu\frac{\partial^2 u_t}{\partial r\partial t}\right) + \eta_3\left(\frac{\partial p}{\partial t} - \mu\frac{\partial^2 u_t}{\partial r^2} - \frac{1}{R}\mu\frac{\partial u_t}{\partial r}\right) + \eta_4\left[-k\left(\frac{\partial^2 T}{\partial r^2} + \frac{\partial^2 T}{\partial t^2}\right) - \mu\left(\frac{\partial u_t}{\partial r}\right)^2\right]\right\}\mathrm{d}\sigma \tag{47}$$

However, for the cost functional (37) we need only the first term in Eq. (47) and, therefore, we choose $\eta_2 = \eta_3 = \eta_4 = 0$:

$$\tilde{\mathcal{L}} + \tilde{\mathcal{L}}_{\mathrm{ABE}} = \text{interior terms} + \int_{\Gamma} 2\tilde{p}(p - p^*)\,\mathrm{d}\sigma$$
$$+ \int_{\partial\Omega} \left[-\tilde{T}k\frac{\partial \boldsymbol{\lambda}_4}{\partial r} + \frac{\partial \tilde{u}_r}{\partial r}\left(\eta_1 + \frac{4}{3}\mu\boldsymbol{\lambda}_r\right) + \frac{\partial \tilde{u}_t}{\partial r}\mu\boldsymbol{\lambda}_t + \tilde{p}\boldsymbol{\lambda}_r \right]\mathrm{d}\sigma$$
$$+ \int_{\Gamma} \tilde{\alpha} g_1(\boldsymbol{U}, \boldsymbol{\Lambda}, \eta_1)\,\mathrm{d}\sigma \tag{48}$$

The variation of the enlarged Lagrangian, $\mathcal{L} + \mathcal{L}_{\mathrm{ABE}}$, yields the following equations on the boundary {using $\tilde{T} = [1/(\gamma - 1)][-(1/\rho^2)\tilde{\rho} + (1/\rho)\tilde{p}]$}:

$$\frac{\partial \tilde{u}_r}{\partial r}(\Gamma): \qquad \eta_1 + \frac{4}{3}\mu\boldsymbol{\lambda}_r = 0$$
$$\tilde{p}(\Gamma): \qquad 2(p - p^*) + \lambda_r - \frac{k}{\gamma - 1}\frac{1}{\rho}\frac{\partial \boldsymbol{\lambda}_4}{\partial r} = 0$$
$$\frac{\partial \tilde{u}_t}{\partial r}(\Gamma): \qquad \mu\boldsymbol{\lambda}_t = 0 \tag{49}$$
$$\tilde{\rho}(\Gamma): \qquad \frac{k}{\gamma - 1}\frac{1}{\rho^2}\frac{\partial \boldsymbol{\lambda}_4}{\partial r} = 0$$

The resulting adjoint equations on the solid wall are given by [see Eq. (35)]

$$\boldsymbol{\lambda}_r = -2(p - p^*), \qquad \boldsymbol{\lambda}_t = 0, \qquad \frac{\mathrm{d}\boldsymbol{\lambda}_4}{\mathrm{d}n} = 0 \tag{50}$$

Note that the first of Eqs. (49) determines the auxiliary Lagrange multiplier η_1

$$\eta_1 = -\tfrac{4}{3}\mu\boldsymbol{\lambda}_r = \tfrac{8}{3}\mu(p - p^*) \tag{51}$$

That Lagrange multiplier is affecting the gradient $g_1 = g_1(\boldsymbol{U}, \boldsymbol{\Lambda}, \eta_1)$ because the variation of the continuity auxiliary boundary equation (40) with respect to a change in the shape Γ results in variational boundary terms that multiply only the term $\tilde{\alpha}$.

V. Conclusion

We present a method for the derivation of the costate equations for problems in which the cost functional does not lead to a proper boundary-value problem for the costate equation, when derived in the standard way. We define such cost functionals as incomplete; it is required to complete the Lagrangian with auxiliary boundary equations in these cases to derive a boundary-value problem of the costate equation. Our aim is to give the costate equations a representation of a boundary-value problem and not to treat rigorously the issue of existence of solutions to the resulting system of costate equations. We demonstrate the method on three problems involving incomplete cost functionals, defined on the boundary, using the potential, the compressible Euler, and the compressible N–S equations. As for cost functionals that are defined in the interior of the domain, we give the following argument: Assume a general cost functional that is defined in the interior of the domain Ω, in terms of the state χ and design α variables:

$$F(\chi, \alpha) = \int_{\Omega} f(D^{k_1}\chi, D^{k_2}\alpha)\,\mathrm{d}x \tag{52}$$

where k_1 and k_2 are positive integers [assuming that χ and α are smooth enough for Eq. (52) to make sense]. After integration by parts the variation of F is given by (again we assume that χ and α are smooth enough for the following equation to make sense)

$$\tilde{F} = \int_{\Omega} \left\{(-1)^{k_1}\tilde{\chi}D^{k_1}\left[f_{D^{k_1}\chi}(D^{k_1}\chi, D^{k_2}\alpha)\right] + (-1)^{k_2}\tilde{\alpha}D^{k_2}\left[f_{D^{k_2}\alpha}(D^{k_1}\chi, D^{k_2}\alpha)\right]\right\}\mathrm{d}x + \text{boundary terms}$$

The interior terms can be matched as usual to form the interior adjoint equations. The boundary terms can be treated with the ABE approach as discussed in the paper.

For nonsmooth problems we make the following comment. The classical Lagrangian formulation used to derive the necessary conditions requires some level of smoothness to apply variational calculus (both for the state variables and for the geometry). For example, a boundary that is C^0 but not C^1 continuous introduces a nontrivial difficulty for that formulation. This is usually resolved by taking contours around the singularities and applying appropriate boundary conditions. This is still true in our approach. Our purpose is to resolve some difficulties within the Lagrangian formulation assuming the same level of smoothness that is required by the classical approach. Our ABE approach does not require more smoothness than the classical approach (and by the definition of the incomplete cost functional).

Finally, we note that for all cost functionals it is possible to derive the adjoint equations in the discrete level in the standard manner; the problem of incompleteness exists only in the PDE level. The strength of our approach is that it enables treatment of a larger class of cost functionals within the continuous adjoint approach. The limitations are the same as for that approach. The relation between the costate equations that we derive and the discretely derived costate equations in the limit of mesh size going to zero is beyond the scope of this paper.

Appendix A: Definition of the Euler Jacobian Matrices

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -u^2 + [(\gamma - 1)/2](u^2 + v^2) & (3 - \gamma)u & -(\gamma - 1)v & \gamma - 1 \\ -uv & v & u & 0 \\ -u[\gamma E - (\gamma - 1)(u^2 + v^2)] & \gamma E - [(\gamma - 1)/2](3u^2 + v^2) & -(\gamma - 1)uv & \gamma u \end{bmatrix} \tag{A1}$$

$$B = \begin{bmatrix} 0 & 0 & 1 & 0 \\ -uv & v & u & 0 \\ -v^2 + [(\gamma - 1)/2](u^2 + v^2) & -(\gamma - 1)u & (3 - \gamma)v & \gamma - 1 \\ -v[\gamma E - (\gamma - 1)(u^2 + v^2)] & -(\gamma - 1)uv & \gamma E - [(\gamma - 1)/2](u^2 + 3v^2) & \gamma v \end{bmatrix} \tag{A2}$$

Appendix B: Identities of Polar Coordinates

$$\text{grad}(f) = \left(\frac{\partial f}{\partial r}, \frac{1}{r}\frac{\partial f}{\partial \theta}\right) \tag{B1}$$

$$\text{div}(\boldsymbol{u}) = \frac{\partial u_r}{\partial r} + \frac{1}{r}\frac{\partial u_t}{\partial \theta} + \frac{u_r}{r} \tag{B2}$$

$$\text{grad}(\boldsymbol{u}) = \begin{pmatrix} \dfrac{\partial u_r}{\partial r} & \dfrac{1}{r}\dfrac{\partial u_r}{\partial \theta} - \dfrac{u_t}{r} \\ \dfrac{\partial u_t}{\partial r} & \dfrac{1}{r}\dfrac{\partial u_t}{\partial \theta} + \dfrac{u_r}{r} \end{pmatrix} \tag{B3}$$

If $A = A_{ij}$ is a tensor, then

$$\text{div} A = \begin{pmatrix} \dfrac{\partial A_{11}}{\partial r} + \dfrac{A_{11}}{r} + \dfrac{1}{r}\dfrac{\partial A_{12}}{\partial \theta} - \dfrac{A_{22}}{r} \\ \dfrac{\partial A_{21}}{\partial r} + \dfrac{A_{21}}{r} + \dfrac{1}{r}\dfrac{\partial A_{22}}{\partial \theta} + \dfrac{A_{12}}{r} \end{pmatrix} \tag{B4}$$

Appendix C: Demonstration of the Adjoint Derivation on a Complex Cost Functional Governed by the Compressible N–S Equations

Let us take, for example, the following cost functional, which is incomplete:

$$F = \int_\Gamma (\rho - \rho^*)^2 \,\mathrm{d}\sigma + \int_\Gamma \left(\frac{\partial p}{\partial n} - f^*\right)^2 \mathrm{d}\sigma \tag{C1}$$

The Lagrangian is given by

$$\begin{aligned} \mathcal{L} &= \int_\Gamma (\rho - \rho^*)^2 \,\mathrm{d}\sigma + \int_\Gamma \left(\frac{\partial p}{\partial n} - f^*\right)^2 \mathrm{d}\sigma \\ &+ \int_\Omega \boldsymbol{\Lambda}^T \cdot (\nabla \cdot \boldsymbol{F}) \,\mathrm{d}\Omega + \int_\Gamma \zeta \frac{\partial T}{\partial n}\sigma \\ &+ \int_\Gamma \iota \cdot \boldsymbol{u}\sigma + \text{far-field terms} \end{aligned} \tag{C2}$$

The variation of the Lagrangian with respect to a change in the shape $\tilde{\alpha}$ is given by

$$\begin{aligned} \tilde{\mathcal{L}} &= \text{interior terms} + \int_\Gamma 2\tilde{\rho}(\rho - \rho^*) \,\mathrm{d}\sigma \\ &+ \int_\Gamma 2\frac{\partial \tilde{p}}{\partial n}\left(\frac{\partial p}{\partial n} - f^*\right) \mathrm{d}\sigma + \int_{\partial\Omega} \left[-\tilde{T}k\frac{\partial \lambda_4}{\partial r} \right. \\ &\left. + \frac{\partial \tilde{T}}{\partial r}k\lambda_4 + \frac{\partial \tilde{u}_r}{\partial r}\frac{4}{3}\mu\lambda_r + \frac{\partial \tilde{u}_t}{\partial r}\mu\lambda_t + \tilde{p}\lambda_r\right] \mathrm{d}\sigma \end{aligned} \tag{C3}$$

For the cost functional (C1), we need only the first two terms in Eq. (47) and, therefore, we choose $\eta_3 = \eta_4 = 0$:

$$\begin{aligned} \tilde{\mathcal{L}}_{\text{ABE}} &= \int_\Gamma \left[\eta_1\left(\frac{\partial \tilde{u}_r}{\partial r}\right) + \eta_2\left(\frac{\partial \tilde{p}}{\partial r} - \mu_2\tilde{\rho}\frac{1}{\rho^2}\frac{\partial \rho}{\partial t}\frac{\partial u_t}{\partial r} \right.\right. \\ &\left.\left. + \mu_2\frac{1}{\rho}\frac{\partial \tilde{\rho}}{\partial t}\frac{\partial u_t}{\partial r} + \mu_2\frac{1}{\rho}\frac{\partial \rho}{\partial t}\frac{\partial \tilde{u}_t}{\partial r} - 2\mu\frac{\partial^2 \tilde{u}_r}{\partial r^2} - \mu\frac{\partial^2 \tilde{u}_t}{\partial r \partial t}\right)\right] \end{aligned} \tag{C4}$$

The term $\partial^2 \tilde{u}_r / \partial r^2$ does not cancel with any other term in the Lagrangian, and therefore, we add another ABE by taking the radial derivative of the continuity equation,

$$\frac{\partial^2}{\partial r^2}(\rho u_r) + \frac{\partial^2}{\partial r \partial t}(\rho u_t) = 0 \tag{C5}$$

and by restricting it to the boundary,

$$\lim_{x \to \Gamma} \frac{\partial}{\partial r}\text{div}(\rho \boldsymbol{u}) = \rho\frac{\partial^2 u_r}{\partial r^2} + \frac{\partial \rho}{\partial t}\frac{\partial u_t}{\partial r} + \rho\frac{\partial^2 u_t}{\partial r \partial t} = 0 \tag{C6}$$

We can further add to the variation of the Lagrangian [Eq. (C3) added with Eq. (C4)] the variation of the residuals of Eq. (C6) with a Lagrange multiplier η_5:

$$\begin{aligned} \tilde{\mathcal{L}}_{\text{new}} &= \tilde{\mathcal{L}} + \tilde{\mathcal{L}}_{\text{ABE}} + \int_\Gamma \eta_5\left(\tilde{\rho}\frac{\partial^2 u_r}{\partial r^2} + \rho\frac{\partial^2 \tilde{u}_r}{\partial r^2}\right. \\ &\left. + \frac{\partial \tilde{\rho}}{\partial t}\frac{\partial u_t}{\partial r} + \frac{\partial \rho}{\partial t}\frac{\partial \tilde{u}_t}{\partial r} + \tilde{\rho}\frac{\partial^2 u_t}{\partial r \partial t} + \rho\frac{\partial^2 \tilde{u}_t}{\partial r \partial t}\right) \mathrm{d}\sigma \end{aligned} \tag{C7}$$

The resulting adjoint equations on the boundary are given by

$$\frac{\partial \tilde{u}_r}{\partial r}(\Gamma): \qquad \eta_1 + \frac{4}{3}\mu\boldsymbol{\lambda}_r = 0$$

$$\frac{\partial^2 \tilde{u}_r}{\partial r^2}(\Gamma): \qquad -2\mu\eta_2 + \eta_5\rho = 0$$

$$\frac{\partial \tilde{p}}{\partial r}(\Gamma): \qquad \eta_2 - 2\left(-\frac{\partial p}{\partial r} - f^*\right) = 0$$

$$\tilde{p}(\Gamma): \qquad \lambda_r - \frac{k}{\gamma - 1}\frac{1}{\rho}\frac{\partial \boldsymbol{\lambda}_4}{\partial r} = 0$$

$$\frac{\partial \tilde{u}_t}{\partial r}(\Gamma): \qquad \mu\lambda_t + \eta_2\mu_2\frac{1}{\rho}\frac{\partial \rho}{\partial t} + \mu\frac{\partial \eta_2}{\partial t} - \frac{\rho\partial\eta_5}{\partial t} = 0$$

$$\begin{aligned} \tilde{\rho}(\Gamma): \qquad & 2(\rho - \rho^*) + \frac{k}{\gamma - 1}\frac{1}{\rho^2}\frac{\partial \boldsymbol{\lambda}_4}{\partial r} - \eta_2\mu_2\frac{1}{\rho^2}\frac{\partial \rho}{\partial t}\frac{\partial u_t}{\partial r} \\ & -\mu_2\frac{\partial}{\partial t}\left(\eta_2\frac{1}{\rho}\frac{\partial u_t}{\partial r}\right) + \eta_5\frac{\partial^2 u_r}{\partial r^2} - \frac{\partial}{\partial t}\left(\eta_5\frac{\partial u_t}{\partial r}\right) + \eta_5\frac{\partial^2 u_t}{\partial r \partial t} = 0 \end{aligned}$$

{We assume that the terms defined on the endpoints of Γ, which result from the integration by parts, are equal to zero and use the relation $\tilde{T} = [1/(\gamma - 1)][-(1/\rho^2)\tilde{\rho} + (1/\rho)\tilde{p}]$.} The preceding system can be solved by first solving for η_1, η_2, and η_5 from the first three equations and then substituting the result in the last three equations, which are the desired adjoint boundary conditions.

Acknowledgments

This research was supported by NASA under Contract NAS1-19480 while the authors were in residence at the Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, Hampton, Virginia. The authors thank Bambang I. Soemarwoto of the Institute of Technology Bandung in Indonesia for fruitful discussions on the derivation of the adjoint equations for the Navier–Stokes equations.

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J. Kallinderis
Associate Editor