On the use of the continuous adjoint method to compute nongeometric sensitivities

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Summary
This work explores an alternative approach to computing sensitivity derivatives of functionals, with respect to a broader range of control parameters. It builds upon the complementary character of Riemann problems that describe the Euler flow and adjoint solutions. In a previous work, we have discussed a treatment of the adjoint boundary problem, which made use of such complementarity as a means to ensure well-posedness. Here, we show that the very same adjoint solution that satisfies those boundary conditions also conveys information on other types of sensitivities. In essence, then, that formulation of the boundary problem can extend the range of applications of the adjoint method to a host of new possibilities.

1 | INTRODUCTION

Over the years, since its extension to transonic flows by Jameson in a landmark work,\textsuperscript{1} the adjoint method has become a veritable field of research in the aerodynamics and Computational Fluid Dynamics (CFD) communities. It has been the subject of extensive investigation and spawned a large variety of applications, ranging from design optimization to flow stability analysis, error estimation and mesh adaptation, and uncertainty quantification.

As a sensitivity analysis tool, the adjoint method allows for efficient computation of the sensitivity derivatives used in design optimization. In a discrete sense, adjoint solutions relate residual perturbations to output perturbations via the chain rule.\textsuperscript{2} While in the continuous sense, adjoint variables correspond to a convolution of the linearized functional and the Green function.\textsuperscript{3,4} Within the sensitivity analyses realm, applications of the method have been mostly focused on optimal geometric shape variations for design optimization and flow stability analyses. In the latter, adjoint solutions are used to calculate the rate of growth of eigenmodes in the flow field.\textsuperscript{5,6}

Another major application of the adjoint method is in estimation and control of discretization errors in outputs via the adjoint-weighted residual method.\textsuperscript{7} In certain types of discretization, adjoint-weighted residual yields consistent estimates of the output error, and the elemental contribution to this error provides an adaptive indicator. With this information, degrees of freedom (DOFs) are added/removed by locally refining/coarsening ($h$-adaptation) the mesh and/or by increasing/decreasing ($p$-adaptation) the scheme’s approximation order.

Yet, for all the prominence they have gained in the literature, the more usual applications of the adjoint method are not the main objective of this work. Instead, its purpose is to consider the use of the method to compute sensitivity derivatives...
of functionals in a slightly broader sense, that is, to include control parameters other than those pertaining to geometry or discretization. Other authors have considered these possibilities in terms of the discrete form of the method. Curiously enough, in the continuous form, Anderson and Venkatakrishnan \(^\text{12}\) mentioned the idea but did not develop it.

Of particular interest to us are the parameters that control inflow and far-field boundary conditions, such as flow direction and stagnation properties, or Mach number. The motivation for the research actually came from our previous study on the Euler adjoint boundary conditions. \(^\text{13}\) In that work, we have pursued an analogy between the flow and adjoint Riemann problems, as a means of ensuring the well-posedness of the latter.

However, that approach turned out to be a formal basis for extending the scope of the sensitivity derivatives, a goal that was achieved by considering our findings in the light of the seminal work by Cacuci and collaborators. Cacuci et al \(^\text{14}\) have formally established the theoretical basis behind the adjoint method of sensitivity analysis for nonlinear systems. Two equally relevant works by the same author followed soon after, with an in-depth analysis of the mathematical foundations underlying the method. The first one \(^\text{15}\) discusses the necessary and sufficient conditions for the existence and uniqueness of adjoint operators, whereas the second \(^\text{16}\) extends the scope of the adjoint formalism to a larger variety of responses, which includes general operators. It is worth adding that, along with his collaborators, the author went on to publish a number of relevant references on a wide range of applications of the method. \(^\text{5,17-25}\)

Two of the above works by Cacuci are especially relevant to our purposes. Cacuci et al \(^\text{14}\) devise a sequence of formal steps to construct the adjoint problem. Whereas, in Cacuci, \(^\text{15}\) conditions for the existence and uniqueness of the adjoint operator require the underlying spaces to be complete and normed (Banach). They also demand that all operators that act upon the state vector admit densely defined partial Gâteaux derivatives with respect to all of their components \(^\text{26}\) and that the Gâteaux differentials be linear in the state vector variations. The need for an inner product is met by further setting the problem in Hilbert spaces, which are self-dual and where Riesz representation theorem ensures the operators uniqueness. \(^\text{27}\) Next, we present a brief account of those works, as they apply to the particular problem in hand, so as to put more emphasis on the formal, mathematical, aspects of proposed approach.

It starts by considering a measure of merit, an objective functional relative to Euler compressible flows. In generic form, it may be written as \(^\text{14}\)

\[
I_0[Q, \alpha] = \int_D F(Q(\chi), \alpha(\chi), \chi) \, d\chi, \tag{1}
\]

where \(Q\) is the state vector, comprising density, linear momentum, and total energy, while \(\chi\) are coordinates of the domain \(D\) in physical space, \(D \subset \mathbb{R}^d\), and \(\alpha\) represents the set of parameters that control the system, \(\alpha \in \mathbb{R}^N\). In generic form, one has

\[
Q(\chi) = [Q_1(\chi), \ldots, Q_k(\chi)]; \quad \chi = (\chi^1, \ldots, \chi^d); \quad \alpha(\chi) = [\alpha_1(\chi), \ldots, \alpha_N(\chi)]. \tag{2}
\]

The state space is taken to be a \(K\)-dimensional Hilbert space \((Q \in H_Q)\) over the scalar field of real numbers \(\mathbb{R}\). Inner products are defined on the basis of domain and surface integrals, respectively:

\[
\langle f, g \rangle \equiv \int_D f(\chi) \cdot g(\chi) \, dV_\chi; \quad \langle f, g \rangle_s \equiv \int_{\partial D} f(\chi) \cdot g(\chi) \, dS_\chi
\]

and a \(L^2\) norm is induced by that product: \(||f||^2 = \langle f, f \rangle\).

Given the well-known properties of Hilbert spaces, and the fact that Gâteaux differentials of the Euler equations and boundary conditions are linear on \(\delta Q\) and \(\delta \alpha\) (Section 2), a unique set of adjoint Euler equations can be promptly derived (Section 3), which fully agrees with the literature on the method.

Under the above conditions, the objective functional \(I_0\), Equation 1, is an application of type \(H_Q \times \mathbb{R}^N \rightarrow \mathbb{R}\), which is defined in the flow domain \(D \subset \mathbb{R}^d\). Cacuci \(^\text{15,16}\) cites a theorem by Vainberg, which gives necessary and sufficient conditions for a generic functional to have Gâteaux differentiable that are linear on the variations. \(^\text{26}\) However, here, we shall a priori confine the scope of the investigation to objective functionals that meet those conditions, that is, those with first variation of the form:

\[
\delta I_0 = \delta I_{0q} + \delta I_{0s} = \langle F_Q', \delta Q \rangle + \langle F'_\alpha, \delta \alpha \rangle, \tag{4}
\]

where \(\delta I_{0q}\) is the physical part and \(\delta I_{0s}\) the parametric part of the total variation.

Again, in generic form, the physical system is governed by a set \(N\) of \(K\) nonlinear PDEs, which, in turn, are subject to a set \(B\) of boundary and initial conditions. In terms of operators, one can write, \(^\text{14}\)
\[ N[Q(\chi), a] = R(\chi, a), \]  
\[ B[Q(\chi), a] = 0, \]  
where the subscript \([\cdot]\) implies that the conditions are imposed on the appropriate domain boundaries \(\partial D\). Then, in principle, one can define an augmented functional that represents the constrained variational problem,

\[ G(Q, a, \phi, \beta, a) = I_a[Q, a] - \langle \phi, N - R \rangle - \langle \beta, B \rangle_s - \langle a, a - a_o \rangle \]  

Usually nonholonomic, the constraints are introduced by the Lagrange multipliers \(\phi, \beta, \) and \(a\), in the last 3 functionals. The first, \(\phi\), imposes the governing equations, and the second, \(\beta\), enforces its boundary conditions, while the third, \(a\), ensures that the control parameters take on a given set of prescribed values \(a = a_o\), which corresponds to the baseline configuration.

Naturally, the variation of \(G\) in Equation 7 depends on that of the governing equations (5) and boundary conditions (6). These have Gâteaux differentials that are given by

\[ L \delta Q = S \delta a, \]  
\[ B_Q' \delta Q = -B_a' \delta a, \]  
where the operators are defined as \(L \equiv N_Q'\) and \(S \equiv R_a' - N_a'\), respectively.\(^{14}\) The first, \(L\), is the linearized form of the governing equations, whereas the second, \(S\), gathers all parameter variations.

The first term on the Right Hand Side (RHS) of (7) is the measure of merit, for which the variation is given by (4). As for the second term, one must compute its Gâteaux derivative and substitute (8) for the corresponding terms. Then, on making use of Gauss theorem, one can transfer the differential operators from the state vector \(Q\) to the Lagrange multiplier \(\phi\). That leads to

\[ -\langle \phi, L \delta Q \rangle = \langle L^* \phi, \delta Q \rangle - P[\phi, \delta Q]_s. \]  

where the term \(P[\phi, \delta Q]_s\) is the bilinear concomitant the operation ensues\(^{14,28}\) and, again, the symbol \([\cdot]\) refers to the domain boundaries \(\partial D\). Furthermore, the first term on the RHS of (10) contains \(L^*\), which is the adjoint operator to \(L\).

Finally, by computing the Gâteaux differentials of the remaining functionals and on combining them with the above results, one obtains the first variation of the augmented functional, \(\delta G\). It reads,

\[ \delta G = -\langle \delta \phi, N - R \rangle - \langle \delta \beta, B \rangle_s - \langle \delta a, a - a_o \rangle + \langle L^* \phi + F_Q', \delta Q \rangle + \]  
\[ -\langle \beta, B_Q' \delta Q \rangle_s - \left[ \langle P_1(\phi), B_Q' \delta Q \rangle_s + \langle B^*(\phi), M \delta Q \rangle_s \right] + \langle F'_a, \delta a \rangle + \]  
\[ + \langle \phi, S \delta a \rangle - \langle a, \delta a \rangle - \langle \beta, B_a' \delta a \rangle_s, \]  

where \(\delta I_o\) has already been replaced by Equation 4. In addition to that, the bilinear concomitant \(P[\phi, \delta Q]_s\) from (10) has been decomposed into the 2 terms within square brackets. Both of them are inner products, only they must be computed over the appropriate boundaries. The first one involves a \(P_1(\phi)\) and the linearized boundary operator \(B_Q' \delta Q\), while the second involves a \(B^*(\phi)\), which represents the adjoint boundary operator, and a term \(M \delta Q\).

The decomposition of \(P\) is not unique, and neither are the definitions of \(P_1\) and \(M\).\(^{14}\) On the contrary, the only restriction that is actually imposed on the procedure is that the operator \(M\) be linearly independent of \(B_Q'\). As a result of this, the very determination of the adjoint boundary problem hinges upon a nonunique decomposition, and it only makes sense that it should be this way. After all, there must be some leeway left to ensure the problem is well-posed.

The augmented functional \(G\) realizes extrema upon the condition that (11) vanishes for arbitrary, albeit realizable, variations of its parameters:

\[ \delta G = 0 \ \forall \ \{ \delta Q, \delta a, \delta \phi, \delta \beta, \delta a \} \in \{ \text{locus of realizability} \}. \]  

That, in turn, requires that the following conditions be met:

1. The equations that govern the physics (5) and their boundary conditions (6) are satisfied. In addition, the control parameters take on the prescribed baseline values, \(a = a_o\). These requirements imply that the first 3 terms of (11) are identically zero.
2. On imposing the condition,

\[ \beta = -P_1(\phi), \]  

\[ \delta a = 0. \]
one drives to zero the sum of the fifth and sixth terms of (11). This particular equation also solves the \( \beta \) in terms of the \( \phi \).

3. The vector \( \phi \) must satisfy the adjoint equation, which is given by

\[
L^* \phi + F_Q^* = 0,
\]

as it appears in the fourth term of (11). The corresponding boundary conditions are given by the operator

\[
B^*(\phi) = 0,
\]

which comes from the seventh term in that equation. Equation 15 determines \( \phi \) at the boundaries, along with the \( \beta \) thereof.

4. The vector \( a \) is specified by the following condition:

\[
\langle a, \delta \alpha \rangle = \langle F'_a, \delta \alpha \rangle + \langle \phi, S \delta \alpha \rangle - \langle \beta, B'_a \delta \alpha \rangle,
\]

which collects all the remaining terms when \( \delta G = 0 \). In fact, this is the realizable part of the sensitivity gradient, \( \delta I_o \), as will be shown next.

To prove the above statement regarding the sensitivity gradient suffices it to recognize that if the governing equations, (5) and (6), are identically satisfied for a given variation \( \Delta G \), of any size, then, from the very definition of \( G \) in (7), it comes that

\[
\Delta G = \Delta I_o - \langle a, \Delta \alpha \rangle
\]

for

\[
\begin{cases}
\Delta G = G(Q_2, \alpha_2; \beta_2, \phi_2) - G(Q_1, \alpha_1; \beta_1, \phi_1) \\
\Delta I_o = I_o(Q_2, \alpha_2) - I_o(Q_1, \alpha_1) \\
\Delta \alpha = \alpha_2 - \alpha_1
\end{cases}
\]

(17)

In particular for an infinitesimal variation \( \Delta G \to \delta G \), under the above conditions and where \( \phi, \alpha \) and \( \beta \) fulfill the above four requirements, there must correspond a stationary value of \( G \). Therefore, one can write

\[
\delta G = \delta I_o - \langle a, \delta \alpha \rangle = 0,
\]

\[
\delta I_o = \langle a, \delta \alpha \rangle,
\]

\[
\delta I_o = \langle F'_a, \delta \alpha \rangle + \langle \phi, (R'_a - N'_a) \delta \alpha \rangle + \langle P_1(\phi), B'_a \delta \alpha \rangle,
\]

(18)

where Equations 13, 16, and the definition of \( S \) have been used. With the above expression (18), one can estimate the sensitivity gradient on the basis of the adjoint solution \( \phi \) and parameter variations \( \delta \alpha \), alone.

It is worth noting here that all physical variations \( \delta Q \) have been successfully removed from the gradient expression. Moreover, the first term on the RHS of (18) is precisely \( \delta I_o \), whereas the second measures the direct effects of \( \delta \alpha \) on the governing equations, and the third does so with respect to their boundary conditions.

2 | THE VARIATIONAL PROBLEM

As was mentioned above, this work is based on a previous study of ours. In fact, it is an extension of Hayashi et al, even though it focuses on an entirely different class of applications. For that reason, we shall make use here of the same notation as before. For it allows one to clearly distinguish among tensor operations that take place in either state, physical or parameter spaces, something that is crucial to the derivations that follow, and which might otherwise be obscured.

Under these conditions, the well-known Euler equations are represented in physical space by

\[
\frac{\partial Q_a}{\partial t} + \frac{\partial f_{a}^{k'}}{\partial x^{k'}} = 0,
\]

(19)

where “primed” indexes \( (x^{k'}) \) imply Cartesian coordinates, and Greek subscripts range from 1 to 5, indicating coordinates in state space: 1 refers to continuity, 2 to 4 to linear momentum, and 5 refers to the energy equation. State \( Q_a \) and flux \( f_{a}^{k'} \) vectors are defined by

\[
Q_a \Rightarrow \left( \frac{\rho u^a}{e} \right); \quad f_{a}^{k'} \Rightarrow \left( \frac{\rho u^a u^{k'} + p g^{k'}}{e + p} u^{k'} \right).
\]

(20)
In particular for the momentum equations, there is a relation between the superscript \( i' \) and the subscript \( a: i' = a - 1 \) for \( 2 \leq a \leq 4 \). The symbol \( e \) represents total energy, \( e = \rho e_i + \mathbf{u} \cdot \mathbf{u}/2 \); \( e_i \) denotes the specific internal energy; and the \( g^{ij} \) stands for the metric tensor, which is the identity matrix in Cartesian coordinates. The set is closed by the ideal gas relation between pressure and internal energy

\[
p = \rho e_i (\gamma - 1).
\]  

(21)

In transformed space (“unprimed” indexes \( z^k \)), the Euler equations are given by\(^{20}\)

\[
J \frac{\partial Q_a}{\partial t} + J \beta^k_i \frac{\partial f^a_i}{\partial z^k} = 0 \quad \Rightarrow \quad \frac{\partial (JQ_a)}{\partial t} + \frac{\partial F^k_a}{\partial z^k} = 0.
\]  

(22)

A tensorial identity\(^{30}\) is crucial to derive their latter form, and it is also implied in the definition of generalized flux vectors \( F^k_a \),

\[
\frac{\partial (J\beta^k_i)}{\partial z^k} = 0 \quad \Rightarrow \quad F^k_a = J\beta^k_i f^a_i.
\]  

(23)

Generalized flux-Jacobian matrices are then defined on the basis of the above (23),

\[
C^k_{a\beta} = J\beta^k_i \frac{\partial f^a_i}{\partial Q^\beta} = J\beta^k_i A^a_{\beta},
\]  

(24)

and they lead to the following form of the generalized Euler equations

\[
\frac{\partial Q_a}{\partial t} + \frac{C^k_{a\beta}}{J} \frac{\partial Q^\beta}{\partial z^k} = 0.
\]  

(25)

Either in this form, or as they appear in (22), the Euler equations can be imposed on the variational problem as realizability constraints.

The applications of interest here mainly concern aerodynamic forces in steady flows, hence the focus on objective functionals that are integrated over the body surface \( (b_w) \), as opposed to domain integrals—needless to say that the former can be recovered from the latter by means of distributions.\(^{31}\) In this framework, the steady form of (22) is imposed on (1), and, according to (7), it yields

\[
G = \int_{b_w} \left( F(Q, \alpha) \left| \frac{dS'}{dS} \right| + \left( \phi_a, \frac{\partial F^k_a}{\partial z^k} \right) \right) dS + \left( \beta, B \right)_s + \left( a, a - a_0 \right).
\]  

(26)

in transformed space. Here, \( I_o \) represents the original measure of merit, while \( I_{c_1}, I_{c_2}, \) and \( I_{c_3} \) indicate the constraint functionals. The vectors \( \phi_a, \beta, \) and \( a \) are the aforementioned Lagrange multipliers. From (4), the first variation of \( I_o \) is explicitly written as

\[
\delta I_o = \left\{ \frac{\partial F}{\partial Q_a} \left| \frac{dS'}{dS} \right|, \delta Q_a \right\}_{b_w} + \left( F, \delta \left| \frac{dS'}{dS} \right| \right)_{b_w},
\]  

(27)

which identifies the ratio of area elements between physical and transformed spaces, \( |dS'/dS| \), as the single control parameter that appears in \( I_o \).

As for the constraint functionals, each one of them shall be considered separately, below. The first, \( I_{c_1} \), involves the variation of the governing equation, which is given by

\[
\frac{\partial}{\partial z^k} (\delta F^k_a) = 0,
\]  

(28)

and the flux variation is obtained by combining Equations 23 and 24, which results in

\[
\delta F^k_a = C^k_{a\beta} \delta Q^\beta + \delta (J\beta^k_i) f^a_i,
\]  

(29)

where the first term represents the physical and the second represents the parametric part of the total variation. The variation of \( I_{c_1} \) makes use of (28) and of Gauss theorem, to yield

\[
\delta I_{c_1} = \left\{ \left( \phi_a, \frac{\partial F^k_a}{\partial z^k} \right) + \left( \phi_a, \delta F^k_an_k \right)_s \right\} - \left\{ \delta F^k_a \left| \frac{1}{J} \frac{\partial (J\phi_a)}{\partial z^k} \right| \right\},
\]  

(30)
where the surface integral defines the bilinear concomitant, \( P[\phi, \delta Q]_b \), and \( n_k \) is the normal unit vector that points inward, into the domain \( D \). The subscript \( S \) refers to its whole boundary, \( \partial D \), which includes the body surface \( b_w \), the far-field \( b_\infty \), and cut-planes \( b_p \). The variations of \( I_c \) and \( I_s \) follow straight from their Gâteaux differentials, as in Equation 11. Now, it must be noted that we are specifically interested in controlling the inflow boundary conditions. Therefore, we shall have

\[
\delta I_c + \delta I_s = \langle \delta \beta, \mathbf{B} \rangle_{s_i} + \langle \beta, \mathbf{B}'_0 \delta \mathbf{Q} \rangle_{s_i} + \langle \beta, \mathbf{B}'_e \delta \alpha \rangle_{s_i} + \langle \delta \mathbf{a} \rangle_{s_i} \tag{31}
\]

where the notation \( \langle \cdot \rangle_{s_i} \) naturally refers to the inflow boundary, that is, the portion of \( b_\infty \) where \( \mathbf{u} \cdot \mathbf{n} > 0 \). The details of the boundary conditions operators \( \mathbf{B} \) and their differentials shall be discussed later, in section 4. Before that, it is important to assemble the variation of the augmented functional (26).

On adding Equations 27, 30, and 31 up, and by separating the surface integrals that make up the bilinear concomitant according to each boundary, one gets

\[
\delta G = \left\langle \phi_{\alpha} \frac{\partial F_{\alpha}}{\partial x^k} \right\rangle + \left\langle \frac{\partial F_{\alpha}}{\partial x^k} \right\rangle + \left\langle \phi_{\alpha}, \mathbf{B} \right\rangle_{s_i} + \left\langle \mathbf{B}'_0 \delta \mathbf{Q} \right\rangle_{s_i} + \left\langle \beta, \mathbf{B}'_e \delta \alpha \right\rangle_{s_i} + \left\langle \delta \mathbf{a} \rangle_{s_i}
\]

\[
\text{where the parametric flux variations at the inflow and outflow portions of the far-field boundary have been collected in the last term on the second line, in the form } s_i \cup s_o \Rightarrow b_\infty. \text{ It has also been assumed that that boundary maps onto a constant coordinate plane, } b_\infty \Rightarrow \xi^2 = 1. \text{ A separation between physical and parametric variations is apparent in the above equation. The terms } a, b, c, d, \text{ and } f \text{ belong in the former group, which gives rise to the adjoint problem. The remaining terms } e, g, h, \text{ and } i \text{ are part of the sensitivity gradient—in Appendix A, the terms } e, g, \text{ and } h \text{ are further simplified.} \tag{34}
\]
3 | THE ADJOINT EULER EQUATION

The adjoint equation is obtained from term $b$, in Equation 34, and it follows the same reasoning that has been amply discussed in the literature.\textsuperscript{13,29,30} It amounts to finding the nontrivial $\phi_a$ that drives that inner product to zero for any arbitrary, albeit realizable, variation $\delta Q$. The procedure gives rise to the steady form of the adjoint equation. The full equation is postulated so as to match the hyperbolic character of the Euler equation itself.

$$\frac{\partial \phi_a}{\partial t} - C_{\rho a}^k \frac{\partial}{\partial x^k} \left( J \phi_a \right) = 0 \quad (35)$$

On comparing the original Euler (25) with the above equation (35), one should note that the flux Jacobian matrix is transposed and has its sign flipped in the latter. For simplicity, the adjoint variable may be redefined so as to take in the transformation Jacobian, $\phi_a \equiv J \phi_a$, which leads to

$$\frac{\partial \phi_a}{\partial t} - C_{\rho a}^k \frac{\partial \phi_a}{\partial x^k} = 0 \quad (36)$$

Clearly, one is only interested in the steady state solution to (36), in the present context. However, the fact that both primal and dual problems share in the same hyperbolic character, with complementary Riemann problems, is at the crux of our approach to the adjoint boundary conditions. It is also the basis for the developments that follow next.

4 | ADJOINT BOUNDARY CONDITIONS

The adjoint boundary problem is formulated on the basis of terms $c$, $d$, and $f$ from Equation 34. Those inner products should be driven to zero, in a manner that is both consistent with flow boundary conditions and with the well-posedness of the adjoint equation. The topic has been discussed at length in Hayashi et al.,\textsuperscript{13} so only the results that are relevant to the present discussion shall be brought up here.

To put them in increasing order of complexity, the cut-planes are certainly the simplest boundary condition. All that is required is the periodicity of the adjoint variables across those planes, in connection with Equation 32.

For solid walls $(b_w)$, the realizability constraint is given by Equation 33. Its introduction into the expression for $\delta G$ (34) gives rise to term $f$, which also involves the objective functional through the derivative $\partial F/\partial Q_p$. The need to drive that term to zero for arbitrary $\delta Q$ is a single wall boundary condition, which can be cast in the form

$$\phi_{(c+1)} J \beta_t^c n_2 = \phi_{(c+1)} n_1 \bigg|_{b_w} = - \frac{\partial F}{\partial Q_p} \frac{\partial Q_p}{\partial p} \left| ds' \right| = - \frac{\partial F}{\partial p} \left| ds' \right| . \quad (37)$$

This condition is coupled with Reuther scheme for extrapolating the adjoint variables at solid walls.\textsuperscript{29} The far-field boundary conditions are obtained from terms $c$ and $d$, which can be cast in the form

$$\Delta_{c_1} + \Delta_{c_2} + \Delta_d = \left( \beta_a \frac{\partial B_a}{\partial Q_p} \delta Q_p \right)_{s_i} + \left( \phi_a A_{u_{\rho_\nu}} \delta Q_p \right)_{s_i} + \left( \phi_a A_{u_{\rho_\nu}} \delta Q_p \right)_{s_i} . \quad (38)$$

where use was made of Equation 24 and $c$ has been split up into 2 terms, so as to associate them with their counterparts in Equation 11. The first term on the RHS, here, corresponds to the fifth one in (11), whereas the second and third terms are both bilinear concomitants, one for the inflow $(s_i)$ and the other for the outflow $(s_o)$ boundaries. For future convenience, they are termed $\Delta_{c_1}, \Delta_{c_2}$, and $\Delta_d$, respectively. The bilinear concomitants, $\Delta_{c_2}$ and $\Delta_d$, must be decomposed in accordance with Equation 11.

Before proceeding any further, though, it should be noted that the adjoint Equation 36 is generalized. It holds in any coordinate system and, particularly, in the Cartesian. The same applies to the boundary conditions that are imposed on cut-planes, solid walls, and the far-field. In the first case, the periodicity requirement remains unchanged, whereas for the other two, Equations 37 and 38 show their Cartesian forms. Hence, we shall pursue here the same reasoning that was discussed in Hayashi\textsuperscript{13} and solve the adjoint problem directly in physical space, which is represented by Cartesian coordinates.
4.1 The 2-D problem

For 2-D flows, the Greek subscripts range from 1 to 4, where 1 refers to continuity, 2 and 3 to linear momentum, and 4 to energy. Latin indexes refer to the 2 dimensions in physical space—for simplicity, \(x'^1 = x\), \(x'^2 = y\). The corresponding flux Jacobian matrices are denoted by \(A'^1 = A\) and \(A'^2 = B\), respectively. Under these circumstances, the adjoint equation becomes

\[
\frac{\partial \phi_{\alpha}}{\partial t} - A_{\beta \alpha} \frac{\partial \phi_{\beta}}{\partial x} - B_{\beta \alpha} \frac{\partial \phi_{\beta}}{\partial y} = 0. 
\]

(39)

The flux Jacobian operator is denoted, \(A_{\beta \alpha} = A\).\(^T\) = \(A\)\(^T\), \(B\) \(B\)\(^T\), for simplicity.\(^32\) Its projection onto the normal direction to a given boundary, \(k = (k_x, k_y)\), defines

\[
-k_{k}^{T} \equiv -A\cdot k = -k_x A^T - k_y B^T, 
\]

(40)

where the minus sign and the transposition, from Equation 39, have been retained for future convenience. The similarity transformation that diagonalizes the resulting matrix yields

\[
-A = -P^T \cdot K_k^{T} \cdot (P^{-1})^T 
\]

(41)

which are obviously the same eigenvalues of the Euler equation, but for the sign reversal. Also associated with the direction \(k\), the similarity transformation operators are given by\(^32\)

\[
P^T = \begin{pmatrix} 1 & u & v & \frac{u u}{2} \\ 0 & \rho k_x & -\rho k_y & \rho \left(\frac{u u}{2} - v k_x\right) \\ \frac{\rho}{\theta} \frac{\rho(k_x + u)}{2} & \frac{\rho(k_y + v)}{2} & \rho \frac{v}{\theta} \left(\frac{v}{\theta} - u n + \frac{u u}{2}\right) \\ \frac{\rho}{\theta} \frac{\rho(k_y - v)}{2} & \frac{\rho(k_x - u)}{2} & \rho \frac{u}{\theta} \left(\frac{v}{\theta} - u n + \frac{u u}{2}\right) \end{pmatrix}, \]

(42)

\[
(P^{-1})^T = \begin{vmatrix} 1 - \frac{(y-1)(u u)}{2c} & \frac{v k_x - v k_y}{\rho} & \frac{(y-1)(u u)}{2c} - \frac{2pc}{\theta} & \frac{(y-1)(u u)}{2c} + \frac{2pc}{\theta} \\ \frac{(y-1)u}{c^2} & \frac{k_x}{\rho} & \frac{c}{\rho} & \frac{c}{\rho} \\ \frac{(y-1)v}{c^2} & \frac{c}{\rho} & \frac{k_y}{\rho} & \frac{c}{\rho} \\ \frac{(y-1)}{c^2} & 0 & \frac{c}{\rho} & \frac{c}{\rho} \end{vmatrix}. \]

(43)

The characteristic form of the adjoint equation is obtained by left multiplying (39) through by \(P^T\), which leads to the expression

\[
P^T \frac{\partial \phi}{\partial t} - P^T A^T (P^{-1})^T P^T \frac{\partial \phi}{\partial x} - P^T B^T (P^{-1})^T P^T \frac{\partial \phi}{\partial y} = 0. 
\]

(44)

It may be added that the product \((P^T \frac{\partial \phi}{\partial t})\) defines adjoint Riemann differentials. Accordingly, on computing the matrix products in Equation 44, one obtains a set of Riemann, or characteristic, equations in the form

\[
\sum_{\beta=1}^{N} K_{\alpha \beta} \frac{\partial \phi_{\beta}}{\partial t} = \sum_{\beta=1}^{N} K_{\alpha \beta} \frac{\partial \phi_{\beta}}{\partial x} + \sum_{\beta=1}^{N} K_{\alpha \beta} \frac{\partial \phi_{\beta}}{\partial y}. 
\]

(45)

where \(N = 4\) and the coefficients \(K_{\alpha \beta}^x\), \(K_{\alpha \beta}^y\), and \(K_{\alpha \beta}^z\) are listed in Table A1, at the end of the paper. The above set keeps the linearity of the original Equation 39. Their only difference lies in that each equation \(\alpha\) from (45) is associated with a particular characteristic velocity, that is, the corresponding eigenvalue from Equation 41.

By picking the vector \(k\) normal to the domain boundaries, those eigenvalues determine which of the adjoint characteristics enter or leave the flow domain. As was discussed in Hayashi et al., domain incoming characteristics are replaced
by boundary conditions, whereas the outgoing ones feed domain information back to the boundary, thus completing the Riemann problem. The equations that represent the latter are picked out from (45), for each case.

### 4.1.1 Solid wall

In a 2-D mapping of type \((x, y) \equiv (\xi, \eta)\), the contour of the body can be specified either as a level curve, such as \(\eta(x, y) = 0\), or in parametric form by \(x(\xi, 0)\) and \(y(\xi, 0)\). In any case, the area element ratio can be written as

\[
\frac{|dS'|}{dS} = \sqrt{\left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2} = \sqrt{g_{11}},
\]

where \(g_{11}\) is an element of the metric tensor \(g_{ij}\). Hence, the solid wall boundary condition from Equation 37 becomes

\[
k_x \varphi_2 + k_y \varphi_3 = \frac{\partial F}{\partial p} \sqrt{g_{11}}.
\]

As it has been discussed at length in Hayashi et al, the above condition must be combined with an extrapolation scheme. In that regard, the aforementioned Reuther scheme suits our applications very well. On representing ghost cells values by \(\varphi^+_k\) and the corresponding values in domain neighboring cells by \(\varphi^-_k\), the equations read

\[
\begin{aligned}
\varphi^-_1 &= \varphi^+_1 \\
\varphi^-_2 &= \varphi^+_2 + \frac{2k_y}{k_x + k_y} \left(\frac{\partial F}{\partial p} \sqrt{g_{11}} - k_x \varphi^+_2 - k_y \varphi^+_3\right) \\
\varphi^-_3 &= \varphi^+_3 + \frac{2k_y}{k_x + k_y} \left(\frac{\partial F}{\partial p} \sqrt{g_{11}} - k_x \varphi^+_2 - k_y \varphi^+_3\right) \\
\varphi^-_4 &= \varphi^+_4
\end{aligned}
\]

and the condition (47) is met at the wall boundary in terms of the average,

\[
k_x \left(\frac{\varphi^-_2 + \varphi^+_2}{2}\right) + k_y \left(\frac{\varphi^-_3 + \varphi^+_3}{2}\right) = \frac{\partial F}{\partial p} \sqrt{g_{11}}.
\]

This scheme has been amply verified in the literature. It has shown to lead to estimates of the sensitivity gradient that are in agreement with those obtained by other methods, within reasonable accuracy levels. Hence, it should be consistent with the proposed applications.

### 4.1.2 Outflow

Outflow boundary conditions come next in increasing order of complexity. The expressions are obtained from term \(d\) in Equations 34 and 38. Since we are mostly interested in external flow applications, this particular boundary is not subject to parametric control. So its bilinear concomitant \(\Delta_d\) should be simply driven to zero.

\[
\Delta_d = \left(\varphi_a A_{\alpha\beta} n^\alpha \delta Q^\beta\right)_{\alpha_i} \Leftrightarrow \left(\varphi^T \cdot n_{K} \cdot \delta Q\right)_{\alpha_i} = 0
\]

The derivation follows the same reasoning from Hayashi et al, so as to remain consistent with the well-posedness of the flow and adjoint equations alike.

The contour problem is rather trivial for supersonic outflows. Since they do not require any physical boundary condition, simple homogeneous adjoint boundary conditions suffice to drive \(\Delta_d\) to zero. Quite differently, subsonic outflows imply the presence of 3 domain incoming adjoint characteristics. They represent the first, second, and fourth eigenvalues in (41), and their corresponding lines in (45) must be replaced by boundary conditions. Hence, it is only the third adjoint characteristic, which is associated with \(- (\mathbf{u} \cdot \mathbf{n} + c)\), that actually needs to be solved.

Therefore, the subsonic outflow requires 3 adjoint boundary conditions. They come from the single realizability constraint that is imposed on \(\delta Q_4\) at that boundary. In the applications of interest here, the static pressure is the only quantity that is fixed at an outflow boundary. On imposing the condition that \(\delta p = 0\), one gets

\[
\delta Q_4 = u \delta Q_2 + v \delta Q_3 = \frac{(u^2 + v^2)}{2} \delta Q_1.
\]

The above equation represents the locus of realizable variations at the outflow boundary. It preserves 3 physical DOFs, since it gives the realizable \(\delta Q_4\) in terms of \(\delta Q_1, \delta Q_2,\) and \(\delta Q_3,\) which should be arbitrary. In essence, preserved physical
DOFs correspond to domain outgoing flow characteristics, and, thus, they represent the flow solution and its arbitrary variations.

On substituting (51) for the corresponding variations in (50), and by requiring it to vanish identically, one obtains the 3 corresponding adjoint boundary conditions:

\[
\begin{align*}
\varphi_1 &= \frac{1}{2} \left[ 2\varepsilon \gamma - (\gamma - 1) \left( u^2 + v^2 \right) \right] \varphi_4 = C_1 \varphi_4 \\
\varphi_2 &= \frac{-2\varepsilon \gamma k_x + (\gamma - 2) k_u u - 2 k_v v \gamma}{2(k_u + k_v)} \varphi_4 = C_2 \varphi_4 \\
\varphi_3 &= \frac{-2\varepsilon \gamma k_x + (\gamma - 2) k_v - 2 k_u u + k_y v}{2(k_u + k_v)} \varphi_4 = C_3 \varphi_4 
\end{align*}
\]

(52)

In terms of operators, Equations 51 and 52 correspond to \( B'_Q \cdot \delta Q = 0 \) and \( B^* \cdot \varphi = 0 \), respectively. The first one comes from Equation 9, and it accounts for the fact that \( B'_n = 0 \) at the outflow. The expressions for \( B'_Q \) and \( B^* \) are given by

\[
\begin{align*}
B'_Q \bigg|_{x_n} &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{-u u}{2} & u & v & -1 \end{pmatrix} ; \\
B^* \bigg|_{x_n} &= \begin{pmatrix} 1 & 0 & 0 & -C_1 \\ 0 & 1 & 0 & -C_2 \\ 0 & 0 & 1 & -C_3 \\ 0 & 0 & 0 & 0 \end{pmatrix} 
\end{align*}
\]

(53)

The first 3 lines of \( B'_Q \) refer to the free DOFs (\( \delta Q_1, \delta Q_2, \) and \( \delta Q_3 \)), which, in turn, correspond to the 3 domain outgoing flow characteristics, whereas the last line of \( B^* \) implies that \( \varphi_3 \) shall be obtained by solving the single outgoing adjoint characteristic, that is, the third.

Under these conditions, the proposed decomposition of the bilinear concomitant in Equation 50 is given by

\[
\begin{align*}
P_1(\varphi) &= -\varphi^T \hat{A}_K \\
B^*(\varphi) &= \varphi^T B^{*T} 
\end{align*}
\]

(54)

Then, on accounting for the fact that \( \Delta_d \) is actually a scalar, and by substituting the above (54) for their counterparts in the expression between square brackets from (11), one gets

\[
\begin{align*}
\langle \varphi^T \cdot \hat{A}_K \cdot \delta Q \rangle &_{x_n} = \langle P_1(\varphi), B'_Q \delta Q \rangle_{x_n} + \langle B^*(\varphi), M \delta Q \rangle_{x_n} \\
&= -\langle \varphi^T \cdot \hat{A}_K \cdot B'_Q \cdot \delta Q \rangle_{x_n} + \langle \varphi^T \cdot B^{*T} \cdot M \cdot \delta Q \rangle_{x_n} \\
\langle \varphi^T \cdot \hat{A}_K \cdot (I + B'_Q) \cdot \delta Q \rangle_{x_n} &= \langle \varphi^T \cdot B^{*T} \cdot M \cdot \delta Q \rangle_{x_n},
\end{align*}
\]

(55)

where \( I \) stands for the identity matrix, and the matrix \( M \) is given by

\[
M \bigg|_{x_n} = \sqrt{g_{11}} \begin{pmatrix} 1 & 0 & 0 \\ -u (u \cdot n) & k_x u + u \cdot n & k_y \\ -v (u \cdot n) & k_x v & u \cdot n + k_y v \\ 0 & 0 & 0 \end{pmatrix}.
\]

(56)

which clearly results in an operator that is linearly independent from \( BQ' \) in Equation 53. Therefore, it proves that the same outflow adjoint boundary conditions, which were shown to be consistent with well-posedness in Hayashi et al., also meet the requirements that have been proposed by Cacuci et al. Therein lies its relevance to next topic, the inflow boundary.

Before moving on to that topic, though, we must turn our attention to the completion of the Riemann problem at the outflow. To that end, the 3 boundary conditions from (52) must be combined with the third adjoint characteristic from (45), in a single set. That could be done either by using the equations as they are or, alternatively, by differentiating (52) with respect to time. In principle, the second option seems to allow for a simpler implementation, so it has been chosen.

On differentiating Equation 52 with respect to time it yields: \( \dot{\varphi}_a = \dot{C}_a \varphi_4 + C_a \dot{\varphi}_4 \), where \( 1 \leq a \leq 3 \) and the dot represents \( \partial / \partial t \). However, in the present context, the coefficients are based on a steady flow solution, so \( \dot{C}_a = 0 \). Hence, the complete set for the Riemann problem at the outflow boundary can be cast in the form
\[
\begin{align*}
\begin{cases}
\dot{\varphi}_1 - C_1 \varphi_4 &= 0 \\
\dot{\varphi}_2 - C_2 \varphi_4 &= 0 \\
\dot{\varphi}_3 - C_3 \varphi_4 &= 0 \\
\left( \sum_{\beta=1}^{3} K_{3\beta} C_\beta + K_{34} \right) \varphi_4 &= R_3 
\end{cases}
\end{align*}
\]

where the spacial derivatives in the RHS of the third characteristics have been collected up in the \( R_3 \) term. The resulting set is amenable to numerical integration by explicit time stepping.

### 4.1.3 Inflow

Because they are subject to parametric control, the inflow boundary conditions are the most complex ones to be considered here. Two terms concern them in Equation 38, they are

\[
\Delta_{c_1} + \Delta_{c_2} = \left\langle \beta_{a_{st}}, \delta Q \right\rangle_{s_i} + \left\langle \varphi_{a_{st}} A^t_{\varphi} n_i, \delta Q \right\rangle_{s_i} \iff \left\langle \beta \cdot B'_Q \cdot \delta Q \right\rangle_{s_i} + \left\langle \varphi^T \cdot \delta Q \right\rangle_{s_i},
\]

and they correspond to the inner product \( c \) in Equation 34. In particular, the second term \( \Delta_{c_2} \) is a bilinear concomitant, and so, it shall be decomposed according to Cacuci et al.\cite{14}

At a supersonic inflow, the primitive variables \( \mathbf{V} \equiv (\rho, u, v, p)^T \) are fully specified, and they fix \( \mathbf{Q} \), which implies that \( \alpha \equiv \mathbf{V} \) and \( \mathbf{B}[\mathbf{Q}, \mathbf{V}] = 0 \). Conversely, the adjoint variables are not imposed any boundary condition, and \( \varphi \) comes from the adjoint solution itself. As a result of that, the flow boundary operator is the identity matrix \( \mathbf{B}'_Q = \mathbf{I} \), and, for lack of any adjoint boundary conditions, one has \( \mathbf{B}^* = 0 \). Therefore, Equation 9 takes on the form

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\delta Q_1 \\
\delta Q_2 \\
\delta Q_3 \\
\delta Q_4
\end{pmatrix} = 
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \rho & 0 & 0 \\
0 & \rho & \rho & 0 \\
\frac{\rho \rho - 1}{(\gamma - 1)} & 0 & 0 & \rho
\end{pmatrix}
\begin{pmatrix}
\delta \rho \\
\delta u \\
\delta v \\
\delta p
\end{pmatrix},
\]

where the square matrix on the RHS clearly represents the operator \(-\mathbf{B}'_Q \equiv -\mathbf{B}'_Q \). Besides, it may be added that, although the variables \( \mathbf{Q} \) and \( \mathbf{V} \) are fixed for each particular flow solution, taken individually, it does not imply that their virtual variations about that solution are necessarily zero. In fact, the flow sensitivity to such virtual variations is precisely the main objective of the investigation.

Under the above circumstances, the proposed decomposition of the bilinear concomitant at a supersonic inflow reads

\[ P_1(\varphi) = \varphi^T \cdot \mathbf{B}'_Q \quad \text{and} \quad \mathbf{B}^*(\varphi) = 0, \]

which leads to

\[ \left\langle \varphi^T \cdot \mathbf{B}'_Q \cdot \delta Q \right\rangle_{s_i} = \left\langle P_1(\varphi), \mathbf{B}'_Q \delta Q \right\rangle_{s_i} + \left\langle \mathbf{B}^*(\varphi), \mathbf{M} \delta Q \right\rangle_{s_i} = \left\langle P_1(\varphi) \cdot \mathbf{B}'_Q \cdot \delta Q \right\rangle_{s_i} \]

\begin{align*}
&= \left\langle \varphi^T \cdot \mathbf{B}'_Q \cdot \mathbf{I} \cdot \delta Q \right\rangle_{s_i} \\
&= \left\langle \varphi^T \cdot \mathbf{B}'_Q \cdot \mathbf{I} \cdot \delta Q \right\rangle_{s_i} \\
&= \left\langle \varphi^T \cdot \mathbf{B}'_Q \cdot \mathbf{I} \cdot \delta Q \right\rangle_{s_i} \]

\end{align*}

Since \( \mathbf{B}^* \) is zero, the operator \( \mathbf{M} \), here, could be any, provided that it is linearly independent from the identity matrix \( \mathbf{B}'_Q \).

Then, from Equation 13, one can solve for \( \beta \), which yields

\[ \beta = -P_1(\varphi) = -\varphi^T \cdot \mathbf{B}'_Q, \]

and, from (58), one gets for \( \Delta_{c_1} + \Delta_{c_2} \):

\[ \left\langle \beta \cdot \mathbf{B}'_Q \cdot \delta Q \right\rangle_{s_i} + \left\langle \varphi^T \cdot \mathbf{B}'_Q \cdot \delta Q \right\rangle_{s_i} = -\left\langle \varphi^T \cdot \mathbf{B}'_Q \cdot \mathbf{I} \cdot \delta Q \right\rangle_{s_i} + \left\langle \varphi^T \cdot \mathbf{B}'_Q \cdot \delta Q \right\rangle_{s_i} = 0. \]

Therefore, it meets the requirements that have been proposed by Cacuci et al.\cite{14} regarding the decomposition of the bilinear concomitant and the cancelation of the 2 terms: \( \Delta_{c_1} + \Delta_{c_2} = 0. \)

Quite differently, at a subsonic inflow boundary, there is only 1 domain incoming adjoint characteristic. For an inward pointing normal, it is the one that is associated with the eigenvalue \(-\left( \mathbf{n} \cdot c \right)\) in (41). Hence, the fourth PDE from set (45) must be replaced by an adjoint boundary condition. The flow, on the other hand, involves 3 domain incoming characteristics, so it requires 3 physical boundary conditions.
In the applications of interest here, the flow direction $\theta$, along with the stagnation pressure $P_o$ and temperature $T_o$, is prescribed. On casting them in terms of state variables, one gets

\[
\begin{align*}
P_o &= B_1(Q_\beta) = \frac{(y-1)2Q_1}{Q_1} \left[ 1 + \frac{(Q_1^2 + Q_2^2)}{y[2Q_1(Q_1^2 + Q_2^2)]} \right]^{(y-1)/2} \\
T_o &= B_2(Q_\beta) = \frac{(y-1)2Q_1}{Q_1} \left[ 2yQ_1 Q_4 - (y - 1) \left( Q_2^2 + Q_3^2 \right) \right] \\
\tan(\theta) &= B_3(Q_\beta) = \frac{Q_2}{Q_2}
\end{align*}
\]

(64)

To make the algebra a bit simpler, we shall hereafter use the notation $\theta \equiv \tan(\theta)$. Then, by writing the above set in the form of Equation 6, one has

\[
\mathbf{B}[\mathbf{Q}, \mathbf{\alpha}] = 0 \Rightarrow \begin{cases} 
B_1(Q_\beta) - P_o & 0 \\
B_2(Q_\beta) - T_o & 0 \\
B_3(Q_\beta) - \theta & 0
\end{cases},
\]

(65)

where the control parameters are precisely the set $\mathbf{\alpha} \equiv (P_o, T_o, \theta)^T$.

The implicit function theorem\textsuperscript{34} shall be used to obtain the linearized form of (65). To remain consistent with the derivations in Hayashi et al.,\textsuperscript{13} $\delta Q_1$ is taken to be the free DOF, that is, the variation that is related to the single domain outgoing flow characteristic, whereas $\delta Q_2, \delta Q_3,$ and $\delta Q_4$ are considered the dependent variations. Under these conditions, one gets for the main Jacobian determinant

\[
\Delta \equiv \frac{\partial (B_1, B_2, B_3)}{\partial (Q_2, Q_3, Q_4)} = -(y - 1)M^2P_o \neq 0,
\]

(66)

and the total differentials for the dependent variations are computed in the form:

\[
\begin{align*}
\delta Q_2 &= -\frac{1}{\Delta} \left[ \frac{\partial (B_1, B_2, B_3)}{\partial (Q_1, Q_3, Q_4)} \delta Q_1 + \frac{\partial (B_1, B_2, B_3)}{\partial (T_o, Q_3, Q_4)} \delta T_o + \frac{\partial (B_1, B_2, B_3)}{\partial (\theta, Q_3, Q_4)} \delta \theta \right], \\
\delta Q_3 &= -\frac{1}{\Delta} \left[ \frac{\partial (B_1, B_2, B_3)}{\partial (Q_2, Q_1, Q_4)} \delta Q_1 + \frac{\partial (B_1, B_2, B_3)}{\partial (Q_2, T_o, Q_4)} \delta T_o + \frac{\partial (B_1, B_2, B_3)}{\partial (Q_2, \theta, Q_4)} \delta \theta \right], \\
\delta Q_4 &= -\frac{1}{\Delta} \left[ \frac{\partial (B_1, B_2, B_3)}{\partial (Q_2, Q_3, Q_1)} \delta Q_1 + \frac{\partial (B_1, B_2, B_3)}{\partial (Q_2, Q_3, T_o)} \delta T_o + \frac{\partial (B_1, B_2, B_3)}{\partial (Q_2, Q_3, \theta)} \delta \theta \right].
\end{align*}
\]

(67)

The results are then arranged as in Equation 9, $\mathbf{B}_Q' \cdot \delta \mathbf{Q} = -\mathbf{B}_\mathbf{\alpha}' \cdot \delta \mathbf{\alpha}$:

\[
\begin{pmatrix}
\frac{\partial Q_2}{\partial Q_1} & 0 & 0 & 0 \\
\frac{\partial Q_2}{\partial Q_3} & -1 & 0 & 0 \\
\frac{\partial Q_2}{\partial Q_4} & 0 & -1 & 0 \\
\frac{\partial Q_2}{\partial T_o} & 0 & 0 & -1
\end{pmatrix}
\begin{pmatrix}
\delta Q_1 \\
\delta Q_2 \\
\delta Q_3 \\
\delta Q_4
\end{pmatrix}
= -
\begin{pmatrix}
\frac{\partial P_o}{\partial Q_1} & 0 & 0 & 0 \\
\frac{\partial P_o}{\partial Q_3} & 0 & 0 & 0 \\
\frac{\partial P_o}{\partial Q_4} & 0 & 0 & 0 \\
\frac{\partial P_o}{\partial T_o} & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
\delta T_o \\
\delta \theta
\end{pmatrix},
\]

(68)

where the partial derivatives come from the corresponding Jacobian determinants in the total differentials, Equation 67. The above operators are given explicitly by

\[
\mathbf{B}_Q' =
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & u - \frac{\gamma p}{\rho/(\gamma u^2 + v^2)} & -1 & 0 \\
0 & v - \frac{\gamma p}{\rho/(\gamma u^2 + v^2)} & 0 & -1 \\
0 & -\rho u^2 + \gamma \rho (\rho + 1) & 0 & -1
\end{pmatrix},
\]

(69)

\[
\mathbf{B}_\mathbf{\alpha}' =
\begin{pmatrix}
0 & 0 & 0 & 0 \\
\frac{\rho u}{M^2 P_o} & \frac{u}{2T_o} \left( \rho - \frac{2p}{\gamma M^2} \right) & \frac{\rho u^2}{\gamma M^2} \\
\frac{\rho v}{M^2 P_o} & \frac{v}{2T_o} \left( \rho - \frac{2p}{\gamma M^2} \right) & \frac{\rho v^2}{\gamma M^2} \\
\frac{(y-1)p}{P_o} & \frac{1}{(y-1)} & -T_o & 0
\end{pmatrix},
\]

(70)
where the first line of both of them simply means that $\delta Q_1$ is free, in that it represents the effects on the boundary of arbitrary variations in the flow domain.

Now, a relevant finding of the present research lies in the fact that the above operator $B'_0$ is exactly equivalent to equation 43 from Hayashi et al,\textsuperscript{13} which is reproduced below for convenience:

$$
\begin{aligned}
\delta Q_2 &= \frac{u}{2} \left[ 2 - \gamma + \gamma^2 - \frac{2(\gamma-1)y}{(u^2+v^2)} \right] \delta Q_1, \\
\delta Q_3 &= \frac{v}{2} \left[ 2 - \gamma + \gamma^2 - \frac{2(\gamma-1)y}{(u^2+v^2)} \right] \delta Q_1, \\
\delta Q_4 &= \frac{1}{2} \left[ -2e(\gamma - 2)\gamma + (\gamma - 1)^2(u^2 + v^2) \right] \delta Q_1.
\end{aligned}
$$

(71)

The only difference between the above coefficients of $\delta Q_1$ and the corresponding elements in $B'_0$ is that the latter, from (69), are written in terms of $p$, whereas the ones listed in Equation 71 are given in terms of the total energy $e$.

In view of the nonuniqueness of the bilinear concomitant decomposition, as was pointed out by Cacuci et al,\textsuperscript{14} the fact that both forms (69) and (71) are fully equivalent poses an interesting question for further investigation. In any case, it has a major consequence in the present context: It implies that the same inflow adjoint boundary condition could be used here. Provided that it could be adequately put in operator form, $B'(\varphi) = 0$. The original form of this condition is given by equations 45 and 46 of Hayashi et al\textsuperscript{13} as follows:

$$
C_1\psi_1 + C_2\psi_2 + C_3\psi_3 + C_4\psi_4 = 0,
$$

(72)

where the coefficients are given by

$$
\begin{aligned}
C_1 &= \left[ 2 - \gamma + \gamma^2 - \frac{2(\gamma-1)y}{(u^2+v^2)} \right] \frac{(k_u+k_v)}{2}, \\
C_2 &= \left[ (2-\gamma^2)k_uu^2+2(1-\gamma)^2k_uv^2 \right. \left. - \frac{(\gamma-1)y(k_uu^2+k_v)}{2} \right] \frac{2(\gamma y-1)[2k_uu+k_v(u^2-v^2)]}{2(u^2+v^2)}, \\
C_3 &= \left[ \frac{y(\gamma-1)k_uu^2+2k_uu^2}{2(u^2+v^2)} + (2(1-\gamma)y)k_uu^2+2(\gamma-1)y(k_uu^2-2k_vu^2) \right] \frac{2(\gamma y-1)}{2(u^2+v^2)}, \\
C_4 &= \left[ (k_u+k_v)(y-1)(u^2+v^2)-2e(\gamma y-1)y \right] \left[ (2-\gamma^2)(u^2+v^2)-2e(\gamma y-1) \right] \frac{4(u^2+v^2)}{4(u^2+v^2)}.
\end{aligned}
$$

(73)

In fact, the operator form of the above equation (72) is quite simple; it reads

$$
B'_0|_{s_i} = \left( \begin{array}{cccc}
1 - \frac{C_i}{C_i} & -\frac{C_i}{C_i} - \frac{C_i}{C_i} \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array} \right),
$$

(74)

which is consistent with the fact that there is only 1 domain incoming adjoint characteristic at a subsonic inflow boundary. The last 3 lines, in turn, represent 3 domain outgoing adjoint characteristics.

Then, by applying to the inflow boundary the exact same decomposition that is presented in Equation 54,

$$
\begin{aligned}
P_1(\varphi) &= -\varphi^T \hat{A}_K, \\
B'(\varphi) &= \varphi^T B' \varphi^T.
\end{aligned}
$$

(75)

The algebra results entirely analogous to that in Equation 55, as expected. The only difference is that the inner products now refer to the inflow boundary ($s_i$), as opposed to the outflow ($s_o$). Other than for that change, the $M$ operator thus obtained

$$
M|_{s_i} = \sqrt{g_{11}} \left( \begin{array}{cccc}
M_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array} \right); \quad M_{11} = (\gamma^2 - \gamma + 2) \left( k_u + k_v \right) - \frac{e(\gamma - 1)y(k_u u + k_v v)}{(u^2 + v^2)}
$$

(76)

is also linearly independent from the corresponding $B'_0$, as can be clearly seen on comparing the above result with Equation 69. From the first equation in (75) and from (13), one gets for $\beta$,

$$
\beta = -P_1(\varphi) = +\varphi^T \cdot \hat{A}_K.
$$

(77)
Finally, on accounting for the fact that $B^*(\phi) = \phi^T B^T = 0$, and by substituting Equations 75 and 77 for the corresponding terms in Equation 58, one gets for $\Delta_{c1} + \Delta_{c2}$:

$$
\langle \beta \cdot B'_Q \cdot \delta Q \rangle_{s_i} + \langle \phi^T \cdot \delta K \cdot \delta Q \rangle_{s_i} = \langle \beta \cdot B'_Q \cdot \delta Q \rangle_{s_i} + \langle P_{1}(\phi), B'_Q \cdot \delta Q \rangle_{s_i}
$$

$$
= \langle \phi^T \cdot \delta K \cdot B'_Q \cdot \delta Q \rangle_{s_i} - \langle \phi^T \cdot \delta K \cdot B'_Q \cdot \delta Q \rangle_{s_i}
$$

$$
= 0,
$$

which identically vanishes, as indeed that sum should.

Above all, what these results show, regarding the treatment of the far-field boundary problem from Hayashi et al., is that not only it is fully consistent with the requirements by Cacuci et al. but it also enables one to extend the scope of the sensitivity derivatives. In the light of these findings, it appears that our previous work just revolves around simpler cases, where Equations 59 and 68 both have $\delta \alpha = 0$ at the inflow. Hence, the extension, to cases where the inflow parameters do vary, shall be the next topic.

However, before that, the completion of the Riemann problem must be presented. To that end, the first 3 adjoint characteristic PDEs from (45) should be solved in conjunction with the single adjoint boundary condition from Equations 72 to 74.

On differentiating (72) with respect to time, it yields $\dot{C}_d \phi_\alpha + C_d \phi_{s_i} = 0$, where $1 \leq \alpha \leq 4$. Here again, the coefficients from (73) are based on a steady flow solution, so $\dot{C}_d = 0$. Then, on joining the resulting equation with the aforementioned characteristic PDEs, one obtains the complete set:

$$
\begin{align*}
K^1_{11} \frac{\partial \psi_1}{\partial t} + K^1_{12} \frac{\partial \psi_2}{\partial t} + K^1_{13} \frac{\partial \psi_3}{\partial t} + K^1_{14} \frac{\partial \psi_4}{\partial t} &= R_1 \\
K^2_{21} \frac{\partial \psi_1}{\partial t} + K^2_{22} \frac{\partial \psi_2}{\partial t} + K^2_{23} \frac{\partial \psi_3}{\partial t} + K^2_{24} \frac{\partial \psi_4}{\partial t} &= R_2 \\
K^3_{31} \frac{\partial \psi_1}{\partial t} + K^3_{32} \frac{\partial \psi_2}{\partial t} + K^3_{33} \frac{\partial \psi_3}{\partial t} + K^3_{34} \frac{\partial \psi_4}{\partial t} &= R_3 \\
C_1 \frac{\partial \psi_1}{\partial t} + C_2 \frac{\partial \psi_2}{\partial t} + C_3 \frac{\partial \psi_3}{\partial t} + C_4 \frac{\partial \psi_4}{\partial t} &= 0
\end{align*}
$$

(79)

where the spacial derivatives from the RHS of (45) have all been collected up in the $R_a$ terms. The resulting set is amenable to numerical integration by explicit time stepping.

As a side note, it may be added that a similar reasoning to the one above could be pursued with respect to the outflow boundary conditions. That would be especially relevant for internal flow applications, such as convergent-divergent nozzles, where the position and strength of the shock wave are sensitive to the back pressure.

## 5 | Computing the Adjoint Gradient

The original form of the sensitivity gradient comes from Equation 34, and it corresponds to the terms $e, g, h$, and $i$, which are reproduced below:

$$
\langle a, \delta \alpha \rangle = -\langle \phi_a, \delta (J\beta_x^{\alpha}) f_{\alpha}^{n_2} n_2 \rangle_{s_i} + \left( \delta (J\beta_x^{\alpha}) f^e_a \frac{\partial (J\phi_a)}{\partial \beta_k} \right)_{s_i} + \left( \delta (J\beta_x^{\alpha}) f_{\alpha}^{n_2} \right)_{s_i} \frac{\partial (J\phi_a)}{\partial \beta_k} + 
$$

$$
- \left( \phi_a, \delta \left( \frac{dS^a}{\partial dS} \right) \right)_{s_i} - \langle p, \phi_a^{(i+1)} \delta (J\beta_x^{\alpha}) n_2 \rangle_{s_i} - \langle \beta, B'_a \delta \alpha \rangle_{s_i}.
$$

(80)

Among them, the first 4 terms on the RHS represent geometrical variations, and they can be further simplified as it is shown in Appendix A. The last term in the above equation is the only one that actually concerns inflow sensitivity. In the absence of geometry variations, it becomes the single surviving term in the sensitivity gradient,

$$
\langle a, \delta \alpha \rangle = -\langle \beta, B'_a \delta \alpha \rangle_{s_i}.
$$

(81)

For supersonic inflows, the operator $B'_a$ comes from Equation 59, whereas $\beta$ is given by Equation 62. Similarly, in the case of subsonic inflows, $B'_a$ is given by Equation 70, whereas $\beta$ comes from Equation 77.

From the equations that are given above, one can either derive integral expressions for the sensitivity derivatives, or, alternatively, one can simply compute them numerically.
TEST RESULTS

This section presents validation test cases performed for internal and external flows. The accuracy of the adjoint nongeometric sensitivities is assessed by comparison with finite difference gradients. Flow and adjoint solutions were computed on unstructured meshes with triangular elements. The numerical simulations have been run with a cell-centered finite volume method and a second order 5-stage Runge-Kutta time-stepping scheme. The dimensionless form of the flow properties is based on a fixed reference state that corresponds to density, \( \rho_{ref} = 1.486 \, \text{kg/m}^3 \); velocity, \( v_{ref} = 320.44 \, \text{m/second} \); and temperature, \( T_{ref} = 357.77 \, \text{K} \). The specific heat ratio \( \gamma = 1.4 \) and gas constant \( R = 2871/\text{kg} \cdot \text{K} \) are the same for all simulations.

Validation tests follow a basic sequence of increasing complexity. The first tests focus on entirely subsonic and entirely supersonic flows, thus avoiding the occurrence of shock waves in the latter case, as well as the transonic regime. A simple flow through a divergent passage, under appropriate inflow and outflow conditions, is used for that purpose. The computational mesh is depicted in Figure 1; it has a symmetry plane at \( y = 0 \), and the upper wall is described by the parabola \( y = 0.3x^2 + 0.3 \), for \( 0 \leq x \leq 1 \).

Both flow and adjoint solutions have attained an accuracy level of \( 10^{-11} \), in terms of the maximum magnitude of the numerical residue. The measure of merit was taken to be an integral of the wall pressure, as a force projected onto the vertical direction (y axis).

Figure 2A,B displays results for sensitivity derivatives that are obtained by the adjoint method and by finite differences, over a range of Mach numbers. The former, 2A, refers to the supersonic flow, whereas the latter, 2B, to the subsonic flow. A comparison between the 2 methods reveals that the differences remain below \( 4.7 \times 10^{-4} \) for all components in the supersonic case and below \( 2.9 \times 10^{-3} \) in the subsonic case.

In increasing order of complexity, next come supersonic flows with shock waves, but where the position and strength of those waves can be determined beforehand. A well-known example of such flows is the diamond profile, with oblique shock waves and Prandtl-Meyer expansion fans. Figure 3 shows gradient results for a diamond profile of unitary chord length and maximum thickness of 10% at half chord, which is at zero angle of attack. Two distinct measures of merit are considered over a range of Mach numbers, \( 1.5 \leq M_{\infty} \leq 2.5 \): Figure 3A depicts sensitivity derivatives of lift \( L \), while Figure 3B presents those for wave drag \( D \). The profile symmetry can be easily recognized in Figure 3A, since the only nonzero derivative is the one with respect to the y component of \( U_{\infty} \), \( \partial L/\partial v \), which implies a change in angle of attack.

In Figure 4 shows results for the same geometry, Mach number range, and measures of merit, \( L \) in Figure 4A and \( D \) in Figure 4B, but at a 2° angle of attack. The computations have attained the same level of accuracy as those of the previous test. As expected, at an angle of attack, the influence of the far-filed variables \( \rho, u, \) and \( p \) on lift are no longer null—although they remain smaller than that of \( v \) itself.

Last, in terms of complexity, come transonic flows with shock waves of varying strength and position. The first case involves the symmetric NACA 0012 at a 1° angle of attack, over a Mach number range: \( 0.5 \leq M_{\infty} \leq 0.9 \). Results for the
sensitivity gradient are presented in Figure 5 for 2 distinct measures of merit, lift $L$ in Figure 5A and pitching moment $M$ in Figure 5B.

It is plain clear that, unfortunately, the sensitivity derivatives at $M_\infty = 0.8$ and 0.9 have not attained the same level of accuracy of the other Mach numbers.

Finally, Figure 6 presents results for an asymmetric airfoil, the RAE 2822, at an angle of attack of 2°. The Mach number range and the objective functionals are the same: lift $L$ in Figure 6A and pitching moment $M$ in Figure 6B.
Quite distinct from the previous case, though, the differences between adjoint and finite differences results remain of roughly the same order throughout the transonic regime. The fact that that happens even in the presence of shock waves, under similar flow conditions, seems to indicate that the lower accuracy of the previous case might be owed to numerical or mesh problems, for one may argue that the position of a normal shock on a smooth contour could be sensitive to local mesh refinement, to some extent. On the other hand, an oblique wave may have the mesh locally refined for it beforehand. At least in principle, then, at this level of accuracy, one may suppose that the results are more strongly affected by the resolution of the shock front than by its presence per se. The superior accuracy of the results for the diamond profile apparently corroborates that hypothesis.

7 CONCLUSIONS

This paper advances a novel application of the General Theory of Sensitivity Analysis, as developed by D.G. Cacuci, to Euler compressible flows. It adopts the continuous form of the adjoint method and builds upon a previous work of ours. That particular work addressed both physical and adjoint boundary conditions in terms of complete and complementary Riemann problems, so as to ensure the well-posedness of the latter. On doing so, it has given rise to an original approach to the adjoint boundary problem that is amenable to Cacuci’s formalism.

Here, a combination of that formalism with our approach enables one to compute sensitivity derivatives other than those related to geometry optimization. It makes use of the same adjoint solution that underlies the latter, and it poses no additional restrictions to measures of merit. Furthermore, these findings apply to both internal and external Euler flows, in subsonic, transonic, and supersonic regimes alike.

As a proof of concept, the present work focuses on simple 2-D flows for the purpose of validation. In that regard, there are still some questions as to the adjoint variables resolution through shock waves, which are now under investigation.
However, in terms of its conceptual foundations, the approach is equally applicable to 3-D flows and, in principle, its extension to those cases should be merely algebraic.

Another aspect that is now under scrutiny is the extension of this approach to unsteady flows. Put together, the extensions to 3-D and time-dependent flows should open up several interesting possibilities of research. Such seems to be the case with the evaluation of stability derivatives in flight dynamics applications.

ACKNOWLEDGEMENTS

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REFERENCES

APPENDIX A: GRADIENT REDUCTION

The gradient terms $e$, $g$, and $h$ from Equation 34, which only concern geometric variations, can be further simplified. Because each single parameter variation is taken to be independent of all the others, any purely geometric variations are considered in the absence of any other parameter changes. Therefore, those terms can be subject to the same simplification that has been proposed by Jamenson and Sangho.\(^{30}\) Under such conditions, Equation 34 is reduced to

$$
\delta G = \left( \delta \phi_\alpha, \frac{\partial F^k_\alpha}{\partial \xi^k} \right) + \left( \delta \beta, \mathbf{B} \right)_b + \left( \delta \mathbf{a}, \mathbf{a} - a_o \right) - \left( \frac{C^k_{a\beta}}{\delta^k} \frac{\partial (J \phi_\alpha)}{\delta^k}, \delta Q_\beta \right)
$$

(a)

$$
+ \left( \beta, \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C^2_{a\beta} n_2, \delta \bar{Q}_\beta \right)_b + \left( \phi_\alpha C^2_{a\beta} n_2, \delta \bar{Q}_\beta \right)_b
$$

(b)

$$
+ \left( \frac{\partial F}{\partial Q_\alpha} \left| \frac{ds'}{ds} \right| + \left[ \phi_{(i+1)} J \beta^2_{i+1} n_2 \right] \frac{\partial \delta}{\partial Q_\alpha}, \delta Q_\alpha \right)_b + \left( \mathbf{a}, \delta \mathbf{a} \right) + \left( \beta, \mathbf{B} \delta \mathbf{a} \right)_b
$$

(c)

$$
+ \int_{b_w} \left( \phi_\alpha \left[ \delta \left( J \beta^2_{p} \right) f^r_\alpha + C^2_{a\beta} \delta Q_\beta \right] n_2 + F \delta \left| \frac{ds'}{ds} \right| + p \phi_{(i+1)} \delta \left( J \beta^2_{p} \right) n_2 \right) dS
$$

(d)

The procedure replaces the 3 terms $e$, $g$, and $h$ by a single integral over $b_w$, which is hereafter termed $j$. In addition to that, 2 new variations are brought in Equation A1. They are $\delta Q_{p}^*$ and $\delta Q_{\beta} = \delta Q_\beta - \delta Q_{p}^*$. The former, $\delta Q_{p}^*$, represents variations in the state variables that are owed to mesh movement $\delta \xi^k$ alone, at a fixed boundary configuration.\(^{30}\) Despite their particular cause, $\delta \xi^k$, they are of the same nature as the original $\delta Q_\beta$, in that they must satisfy an equation that is fully analogous to the Euler’s.
TABLE A1 Coefficients of the adjoint characteristics equations (45), reproduction from Hayashi et al.\textsuperscript{13}

<table>
<thead>
<tr>
<th>Coef.</th>
<th>Value</th>
<th>Coef.</th>
<th>Value</th>
</tr>
</thead>
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<td>$K_{31}^x$</td>
<td>$\rho (u + k_c v)$</td>
</tr>
<tr>
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<td>$u$</td>
<td>$K_{32}^x$</td>
<td>$[\rho c^2 k_y^2 + \rho (u + k_c v)^2]$</td>
</tr>
<tr>
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<td>$K_{33}^x$</td>
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<tr>
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</tr>
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<tr>
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<td>$[\rho c^2 k_y^2 + \rho (u - k_c v)^2]$</td>
</tr>
<tr>
<td>$K_{23}^r$</td>
<td>$-\rho k_x$</td>
<td>$K_{43}^x$</td>
<td>$- [\rho c^2 k_x k_y - \rho (u - k_c) (v - k_c)]$</td>
</tr>
<tr>
<td>$K_{24}^r$</td>
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<td>$K_{44}^x$</td>
<td>$[\rho c^2 k_x (k_x v - k_x u) + \rho c^2 (u - k_c) (u^2 + v^2)]$</td>
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<tr>
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<td>$v^2$</td>
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<td>$\rho c^2 (u^2 + v^2)/2$</td>
<td>$K_{14}^y$</td>
<td>$- [\rho c^2 (u^2 + v^2)/2 + \rho c^2 (u + k_c c) (u^2 + v^2)]$</td>
</tr>
<tr>
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</tr>
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<td>$K_{42}^y$</td>
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</tr>
<tr>
<td>$K_{24}^x$</td>
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<td>$K_{44}^y$</td>
<td>$[\rho c^2 (u^2 + v^2)/2 + \rho c^2 (v - k_c c) (u^2 + v^2)]$</td>
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