

Non-Geometric Sensitivities Using the Adjoint Method

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Abstract—The adjoint method has been used as a successful tool to obtain sensitivity gradients in aerodynamic design and optimisation for many years. This work presents an alternative approach to the continuous adjoint formulation that enables one to compute gradients of a given measure of merit with respect to control parameters other than those pertaining to geometry. The procedure is then applied to the steady 2-D compressible Euler and incompressible Navier–Stokes flow equations. Finally, the results are compared with sensitivities obtained by finite differences and theoretical values for validation.

Keywords—Adjoint method, optimisation, non-geometric sensitivities, boundary conditions.

I. INTRODUCTION

IT is widely recognised that the use of CFD has made an extraordinary impact on virtually all branches of fluid mechanics. Traditionally, CFD resources have played a crucial part in the analysis of flow physics, thus fulfilling functions that are complementary to those of wind-tunnel testing. More recently, though, the development of algorithms and enhancement of computational power have opened up new possibilities, thus enabling one to explore the design space more efficiently and to achieve more elaborate design goals.

The adjoint method has played a prominent role in that context, for a number of reasons. Among them one could cite the great flexibility it offers with regard to the flow-physics model and to the definition of objective functionals. Originally proposed by Pirronneau [1] for elliptic problems, it was later extended to transonic flows by Jameson [2]. Over the years, it has become the subject of extensive research activity [3], [4], [5], [6], [7], [8], [9], [10], and spawned a wide variety of applications, ranging from nuclear reactor thermal-hydraulics to atmospheric sciences [11], [12].

In aerodynamics, the developments of the adjoint method encompass design applications regarding internal and external flows [13], [14], [15], [16] and, more recently, unsteady flows [17], [18], [19], [20]. An entirely different area of research has evolved around the ideas of error analysis [21], [22] and grid adaptation [23], [24], [22], [25]. It makes use of the adjoint variables to improve the accuracy of functionals, which measure desired qualities of the flow solution [26], [27], [28], [29].

Despite all the developments about the adjoint method listed above, there are some research fields that have not been well explored in the literature. The idea presented in this work, for example, was originally proposed by Cacuci *et al.* [11]

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in a seminal reference to compute general sensitivities in a transient problem in fast reactor thermal hydraulics. On using this approach to aerodynamic applications, one could compute important non-geometric sensitivity derivatives, as those related to inflow boundary conditions. In what follows, a brief account of that material is presented, the reader is referred to the original paper [11] for further details.

II. SENSITIVITY THEORY FOR GENERAL SYSTEMS

Objective functionals of general interest in aerodynamics depend on flow variables and on the shape and location of the boundaries [30], [31]. Initially, one takes a measure of merit of a given physical system in generic form:

$$I_o[\mathbf{Q}, \alpha] = \int_{\chi} \mathcal{F}[\mathbf{Q}(\chi), \alpha(\chi), \chi] d\chi \quad (1)$$

where the vector \mathbf{Q} represents the coordinates of that system in state space. The vector χ gives coordinates in phase space of the points in the domain of interest — in the applications that are considered here, it corresponds to the physical space. Finally, vector α represents the set of parameters that control the system. In generic form, one would have

$$\mathbf{Q}(\chi) = [Q_1(\chi), \dots, Q_K(\chi)] \quad (2)$$

$$\chi = (\chi_1, \dots, \chi_J) \quad (3)$$

$$\alpha(\chi) = [\alpha_1(\chi), \dots, \alpha_I(\chi)] \quad (4)$$

on defining inner products of the form:

$$\langle \Phi, \Psi \rangle = \int_{\mathcal{D}} \Phi \cdot \Psi d\chi \quad ; \quad \langle \Phi, \Psi \rangle_s = \int_{\partial \mathcal{D}} \Phi \cdot \Psi d\chi \quad (5)$$

in the physical domain and on its boundaries, respectively.

The first Gâteaux variation [32] of the functional (1) yields the expression,

$$\delta I_o = \underbrace{\langle \mathcal{F}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle}_{\delta I_{oQ}} + \underbrace{\langle \mathcal{F}'_{\alpha}, \delta \alpha \rangle}_{\delta I_{o\alpha}} \quad (6)$$

where the first term on the RHS, δI_{oQ} , corresponds to the physical part of the total variation, whereas the second, $\delta I_{o\alpha}$, represents the parametric part, in the applications of interest here. In general, the term $\mathcal{F}'_{\alpha} \delta \alpha(\chi)$ is known in closed form and, thus, the variation $\delta I_{o\alpha}$ can be evaluated analytically. The greatest difficulty in estimating δI_o lies in the first term, δI_{oQ} , instead. For the variation $\delta \mathbf{Q}(\chi)$ is seldom known in closed form, even though $\mathcal{F}'_{\mathbf{Q}}$, itself, may be. In effect, the mere presence of δI_{oQ} in the total variation is indicative of

the need for additional flow simulations, as the finite difference method requires.

The need for additional flow simulations could be avoided, if one could ensure that all physical variations $\delta\mathbf{Q}(\chi)$ are realizable. This is exactly what the adjoint method does by imposing the governing equations as realizability constraints to the variational problem. In order to do it, consider that the system is governed by a set \mathbf{N} of K nonlinear PDE's, which, in turn, are subject to a set \mathbf{B} of boundary conditions. In terms of operators,

$$\mathbf{N}[\mathbf{Q}(\chi), \alpha] = \mathbf{R}(\chi, \alpha) \quad (7)$$

$$\mathbf{B}[\mathbf{Q}(\chi), \alpha]_s = 0 \quad (8)$$

Then, one can define the augmented functional:

$$G(\mathbf{Q}, \alpha, \Phi, \beta, a) = I_o(\mathbf{Q}, \alpha) - \langle \Phi, \mathbf{N} - \mathbf{R} \rangle + \langle \beta, \mathbf{B} \rangle_s - \langle \mathbf{a}, \alpha - \alpha_o \rangle \quad (9)$$

Usually non-holonomic, the constraints are introduced by the Lagrange multipliers Φ , β and \mathbf{a} , in the last three functionals of (9). The first of them imposes the governing equations, while the second enforces the corresponding boundary conditions, and the third ensures that the control parameters take on a given set of prescribed values $\alpha = \alpha_o$, which corresponds to a baseline configuration.

In order to determine the extrema of G , it is necessary to compute its variation, δG . To achieve this goal, consider that the Fréchet differentials of equations (7) and (8) are given by:

$$\mathbf{L}\delta\mathbf{Q} = \mathbf{S}\delta\alpha \quad (10)$$

$$\mathbf{B}'_Q\delta\mathbf{Q} = -\mathbf{B}'_\alpha\delta\alpha \quad (11)$$

where the operator $\mathbf{L} \equiv \mathbf{N}'_Q$ is the linearized form of the governing equations, whereas $\mathbf{S} \equiv \mathbf{R}'_\alpha - \mathbf{N}'_\alpha$, corresponds to variations of control parameters. Finally, by computing the Gâteaux variations of the remaining functionals and on combining them with the above results, one obtains the first variation of the augmented functional, δG :

$$\delta G = \langle \mathcal{F}'_Q, \delta\mathbf{Q} \rangle + \langle \mathcal{F}'_\alpha, \delta\alpha \rangle - \langle \delta\Phi, \mathbf{N} - \mathbf{R} \rangle + \langle \Phi, \mathbf{L}\delta\mathbf{Q} \rangle + \langle \Phi, \mathbf{S}\delta\alpha \rangle - \langle \delta\beta, \mathbf{B} \rangle_s - \langle \beta, \mathbf{B}'_Q\delta\mathbf{Q} \rangle_s + \langle \beta, \mathbf{B}'_\alpha\delta\alpha \rangle_s - \langle \delta a, \alpha - \alpha_o \rangle - \langle \mathbf{a}, \delta\alpha \rangle \quad (12)$$

Then, on making use of Gauss' theorem, one can transfer the differential operators from the state vector \mathbf{Q} to the Lagrange multiplier Φ as:

$$\langle \Phi, \mathbf{L}\delta\mathbf{Q} \rangle = \langle \mathbf{L}^*\Phi, \delta\mathbf{Q} \rangle - P[\Phi, \delta\mathbf{Q}]_s \quad (13)$$

where the term $P[\Phi, \delta\mathbf{Q}]_s$ is the bilinear concomitant the operation ensues [11], [33]. It is seen as an inner product between Φ and $\delta\mathbf{Q}$ and gives rise to the adjoint boundary conditions $\mathbf{B}^*(\Phi) = 0$. Furthermore, the first term on the RHS of (13) contains \mathbf{L}^* , which is the adjoint operator to \mathbf{L} .

On combining terms in a convenient way, one has:

$$\delta G = -\langle \delta\Phi, \mathbf{N} - \mathbf{R} \rangle - \langle \delta\beta, \mathbf{B} \rangle_s - \langle \delta a, \alpha - \alpha_o \rangle + \langle \mathbf{L}^*\Phi - \mathcal{F}'_Q, \delta\mathbf{Q} \rangle - \langle \beta, \mathbf{B}'_Q\delta\mathbf{Q} \rangle_s + \left[\langle P_1(\Phi), \mathbf{B}'_Q\delta\mathbf{Q} \rangle_s + \langle \mathbf{B}^*(\Phi), \mathbf{A}\delta\mathbf{Q} \rangle_s \right] + \langle \mathcal{F}'_\alpha, \delta\alpha \rangle + \langle \Phi, \mathbf{S}\delta\alpha \rangle - \langle \mathbf{a}, \delta\alpha \rangle - \langle \beta, \mathbf{B}'_\alpha\delta\alpha \rangle_s \quad (14)$$

where the bilinear concomitant $P[\Phi, \delta\mathbf{Q}]_s$ of (13) has been decomposed into two inner products within square brackets. Both of them must be computed over the appropriate boundaries. The first of them involves $P_1(\Phi)$ and the linearized boundary operator $\mathbf{B}'_Q\delta\mathbf{Q}$, whereas the second involves the adjoint boundary operator $\mathbf{B}^*(\Phi)$ and $\mathbf{A}\delta\mathbf{Q}$. The decomposition of P is **not** unique, and neither are the definitions of P_1 and \mathbf{A} . On the contrary, the only restriction that is actually imposed on the procedure is that the operator \mathbf{A} be linearly independent of \mathbf{B}'_Q .

The augmented functional G realizes extrema upon the condition that (14) vanishes for arbitrary, albeit realizable, variations of its parameters:

$$\delta G = 0 \quad \forall \{ \delta\mathbf{Q}, \delta\alpha, \delta\Phi, \delta\beta, \delta\mathbf{a} \} \in \{ \text{locus of realizability} \} \quad (15)$$

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

- I. The flow governing equations (7) and their respective boundary conditions (8) are satisfied. In addition, the control parameters should take on the prescribed baseline values, $\alpha = \alpha_o$. These requirements imply that the first three terms of (14) are identically zero.
- II. On imposing the condition,

$$\beta = -P_1(\Phi) \quad , \quad (16)$$

one drives to zero the sum of the fifth and sixth terms of (14). This particular equation also solves the β in terms of the Φ .

- III. The vector Φ must satisfy the adjoint equation, which is given by:

$$\mathbf{L}^*\Phi - \mathcal{F}'_Q = 0 \quad , \quad (17)$$

as it appears in the fourth term of (14). The corresponding boundary conditions are given by the operator

$$\mathbf{B}^*(\Phi) = 0 \quad , \quad (18)$$

which comes from the seventh term in that equation. Equation (18) should determine the Φ at the boundaries, along with the β thereof.

- IV. The vector \mathbf{a} is specified by the following condition:

$$\langle \mathbf{a}, \delta\alpha \rangle = \langle \mathcal{F}'_\alpha, \delta\alpha \rangle + \langle \Phi, \mathbf{S}\delta\alpha \rangle - \langle \beta, \mathbf{B}'_\alpha\delta\alpha \rangle_s \quad (19)$$

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

To prove the above statement regarding the sensitivity gradient [11], suffices it to recognize that: If the governing equations (7) and (8) are identically satisfied for a given variation ΔG , of any size. Then, from the definition of G in (9):

$$\Delta G = \Delta I_o - \langle \mathbf{a}, \Delta\alpha \rangle \quad \text{for} \quad \begin{cases} \Delta G \equiv G(Q_2, \alpha_2; \Phi_2, \beta_2, a_2) - G(Q_1, \alpha_1; \Phi_1, \beta_1, a_1) \\ \Delta I_o \equiv I_o(Q_2, \alpha_2) - I_o(Q_1, \alpha_1) \\ \Delta\alpha \equiv \alpha_2 - \alpha_1 \end{cases} \quad (20)$$

In particular for an infinitesimal variation $\Delta G \rightarrow \delta G$, under the above conditions and where Φ , α and β fulfill the above

requirements I–IV, there must correspond a stationary value of G . Therefore, one can write

$$\begin{aligned} \delta G &= \delta I_o - \langle \mathbf{a}, \delta \alpha \rangle = 0 \\ \delta I_o &= \langle \mathcal{F}'_\alpha, \delta \alpha \rangle + \langle \Phi, (\mathbf{R}'_\alpha - \mathbf{N}'_\alpha) \delta \alpha \rangle + \langle P_1(\Phi), \mathbf{B}'_\alpha \delta \alpha \rangle_s \\ \delta I_o &= \langle \mathbf{a}, \delta \alpha \rangle \end{aligned} \quad (21)$$

where (16), (19) and the definition of \mathbf{S} have been used. With the above expression (21), one can estimate the sensitivity gradient on the basis of the adjoint solution Φ and parameter variations $\delta \alpha$, alone.

III. COMPRESSIBLE EULER FORMULATION

The rationale behind the adjoint method consists of separating physical from geometric variations. On doing so, one can eliminate physical variations by solving the adjoint problem. To that end, it is convenient to write the governing equations in terms of generalized coordinates. Equation (22) bellow presents the well-known Euler equations written in this form [34]:

$$\frac{\partial Q_\alpha}{\partial t} + \frac{\partial F_\alpha^k}{\partial \xi^k} = 0 \quad (22)$$

ξ^k represents the generalized coordinates. The state Q_α and flux $f_\alpha^{k'}$ vectors are defined by:

$$Q_\alpha \Rightarrow \begin{pmatrix} \rho \\ \rho u^{i'} \\ e \end{pmatrix} ; \quad f_\alpha^{k'} \Rightarrow \begin{pmatrix} \rho u^{k'} \\ \rho u^{i'} u^{k'} + p g^{i'j'} \\ (e+p)u^{k'} \end{pmatrix} \quad (23)$$

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 $g^{i'j'}$ stands for the metric tensor.

On applying the procedure described in the previous section to the steady form of (22), one obtains the following expression for δG :

$$\begin{aligned} \delta G &= \underbrace{\left\langle \delta \phi_\alpha, \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle + \langle \delta \beta, \mathbf{B} \rangle_{s_i} + \langle \delta \mathbf{a}, \alpha - \alpha_o \rangle +}_{(a)} \\ &- \underbrace{\left\langle \frac{C_{\alpha\beta}^k}{J} \frac{\partial (J\phi_\alpha)}{\partial \xi^k}, \delta Q_\beta \right\rangle}_{(b)} - \underbrace{\left\langle \delta (J\beta_{i'}^2), \frac{f_\alpha^{i'}}{J} \frac{\partial (J\phi_\alpha)}{\partial \xi^k} \right\rangle}_{(c)} + \\ &+ \underbrace{\left\langle \beta_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^2 n_2, \delta Q_\beta \right\rangle}_{(d)}_{s_i} + \\ &+ \underbrace{\left\langle \phi_\alpha C_{\alpha\beta}^2 n_2, \delta Q_\beta \right\rangle}_{(e)}_{s_o} + \underbrace{\left\langle \phi_\alpha, \delta (J\beta_{i'}^2) f_\alpha^{i'} n_2 \right\rangle}_{(f)}_{b_\infty} + \\ &+ \underbrace{\left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right| + [\phi_{(i'+1)} J\beta_{i'}^2 n_2] \frac{\partial p}{\partial Q_\alpha}, \delta Q_\alpha \right\rangle}_{(g)}_{b_w} + \\ &+ \underbrace{\left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle}_{(h)}_{b_w} + \underbrace{\left\langle p, [\phi_{(i'+1)} \delta (J\beta_{i'}^2) n_2] \right\rangle}_{(h)}_{b_w} \end{aligned}$$

$$+ \underbrace{\langle \mathbf{a}, \delta \alpha \rangle + \langle \beta, \mathbf{B}'_\alpha \delta \alpha \rangle}_{(i)}_{s_i} \quad (24)$$

where $\beta_{i'}^k$ is the transformation operator between the Cartesian and the transformed space, $f_\alpha^{i'}$ corresponds to Cartesian flux vectors and $C_{\alpha\beta}^k$ are generalized flux Jacobian matrices. The parametric flux variations at the inflow and outflow portions of the farfield boundary have been collected in the term f using: $s_i \cup s_o \Rightarrow b_\infty$. It has also been assumed that that boundary maps onto a constant coordinate plane, $b_\infty \Rightarrow \xi^2 = 1$. A separation between physical and parametric variations is apparent in the above equation. The terms a, b, d, e and g belong in the former group, which gives rise to the adjoint problem. The remaining terms c, f, h and i are part of the sensitivity gradient and are reproduced below:

$$\begin{aligned} \langle \mathbf{a}, \delta \alpha \rangle &= - \left\langle \phi_\alpha, \delta (J\beta_{i'}^2) f_\alpha^{i'} n_2 \right\rangle_{b_\infty} - \left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle_{b_w} \\ &- \left\langle p, [\phi_{(i'+1)} \delta (J\beta_{i'}^2) n_2] \right\rangle_{b_w} - \langle \beta, \mathbf{B}'_\alpha \delta \alpha \rangle_{s_i} + \\ &+ \left\langle \delta (J\beta_{i'}^k), \frac{f_\alpha^{i'}}{J} \frac{\partial (J\phi_\alpha)}{\partial \xi^k} \right\rangle \end{aligned} \quad (25)$$

Among them, only the fourth term on the RHS of (25) concerns inflow sensitivity. The others represent geometrical variations, and they can be further simplified [35]. In the absence of geometry variations, the gradient becomes:

$$\langle \mathbf{a}, \delta \alpha \rangle = - \langle \beta, \mathbf{B}'_\alpha \delta \alpha \rangle_{s_i} \quad (26)$$

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. In any case, it is worth adding that neither form depends explicitly on the measure of merit. On the contrary, all influence of that functional, which they must certainly bear, comes through the adjoint solution itself.

A. Adjoint Boundary Conditions

It is clear in (26) that the gradient expression depends explicitly on the adjoint variables at inflow boundaries. Hence the traditional homogeneous conditions would erase an invaluable piece of sensitivity information at that boundary, even though they would drive the bilinear concomitant to zero, as expected. In order compute these inflow sensitivities, it is necessary to solve the contour problem in terms of characteristics equations. In particular for Euler flows, both fluid dynamics and adjoint equations entail complementary Riemann problems, and these yield boundary conditions that are fully consistent with well-posedness [34].

On comparing the adjoint boundary conditions terms d, e and h from (26) with the usual adjoint formulation [34], one can realize that only the inflow term d is new. For this reason, it will be our focus here.

Since the flow regime defines the boundary problem, we consider first the supersonic case, where all primitive variables $\mathbf{V} = (\rho, u, v, p)^T$ are fully specified. Conversely, the ϕ are free at inflow boundaries and comes from the adjoint solution. As

a result, the adjoint boundary operator \mathbf{B}^* is the null matrix, while \mathbf{B}'_Q is the identity matrix, and (11) becomes:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \delta Q_1 \\ \delta Q_2 \\ \delta Q_3 \\ \delta Q_4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ u & \rho & 0 & 0 \\ v & 0 & \rho & 0 \\ \frac{\mathbf{u}\cdot\mathbf{u}}{2} & \rho u & \rho v & \frac{1}{(\gamma-1)} \end{pmatrix} \begin{pmatrix} \delta \rho \\ \delta u \\ \delta v \\ \delta p \end{pmatrix} \quad (27)$$

where the square matrix on the RHS clearly represents the operator $-\mathbf{B}'_\alpha \equiv -\mathbf{B}'_V$. 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.

Notice that the condition $\mathbf{B}^*(\Phi) = 0$ drives to zero the second term of the bilinear concomitant decomposition $\langle \mathbf{B}^*(\Phi), \mathbf{A}\delta\mathbf{Q} \rangle$, as can be seen in (14). It also enables one to choose any \mathbf{A} that is linearly independent of \mathbf{B}'_Q so as to satisfy Cacuci's requirement. Finally, from (27) the matrix \mathbf{B}'_α can be obtained for supersonic flows controlled by primitive variables at inflow boundaries:

$$\mathbf{B}'_\alpha = - \begin{pmatrix} 1 & 0 & 0 & 0 \\ u & \rho & 0 & 0 \\ v & 0 & \rho & 0 \\ \frac{\mathbf{u}\cdot\mathbf{u}}{2} & \rho u & \rho v & \frac{1}{(\gamma-1)} \end{pmatrix} \quad (28)$$

For subsonic flows, there is only one incoming adjoint characteristic. The conditions that are usually prescribed are: flow direction, $\vartheta = \tan \theta$; stagnation pressure, p_o ; and temperature, T_o . On writing them in terms of conservative variables \mathbf{Q} and setting their variations to zero, one can obtain three equations for the allowed physical variations, say δQ_2 , δQ_3 and δQ_4 as a function of the remaining δQ_1 . Then, on taking the quantities that are imposed as boundary conditions to be the control parameters, one gets the relation $\mathbf{B}'_Q \delta \mathbf{Q} = -\mathbf{B}'_\alpha \delta \alpha$:

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial Q_1} & -1 & 0 & 0 \\ \frac{\partial Q_3}{\partial Q_1} & 0 & -1 & 0 \\ \frac{\partial Q_4}{\partial Q_1} & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \delta Q_1 \\ \delta Q_2 \\ \delta Q_3 \\ \delta Q_4 \end{pmatrix} = - \begin{pmatrix} 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial p_o} & \frac{\partial Q_2}{\partial T_o} & \frac{\partial Q_2}{\partial \vartheta} \\ \frac{\partial Q_3}{\partial p_o} & \frac{\partial Q_3}{\partial T_o} & \frac{\partial Q_3}{\partial \vartheta} \\ \frac{\partial Q_4}{\partial p_o} & \frac{\partial Q_4}{\partial T_o} & \frac{\partial Q_4}{\partial \vartheta} \end{pmatrix} \begin{pmatrix} \delta p_o \\ \delta T_o \\ \delta \vartheta \end{pmatrix} \quad (29)$$

This procedure leads precisely to the same expressions that are proposed by [34]. It implies that the same inflow adjoint condition can be used here. On substituting the variation $\delta \mathbf{Q}$ from the LHS of (29) to the inflow boundary condition term $\langle \beta, \mathbf{B}'_Q \delta \mathbf{Q} \rangle_{S_i}$ in (14), one can choose β that forces this term to vanish. It results in an expression in the form:

$$C_1 \phi_1 + C_2 \phi_2 + C_3 \phi_3 + C_4 \phi_4 = 0 \quad (30)$$

where, C_i are coefficients that depend only on flow properties. In operator form, one gets the adjoint boundary conditions $\mathbf{B}^*(\Phi) = 0$, that correspond to a locus in state space where the adjoint vector is normal to all realizable variations: $\Phi \perp \delta \mathbf{Q}$.

And the \mathbf{B}'_α matrix becomes:

$$\mathbf{B}'_\alpha = \begin{pmatrix} 0 & 0 & 0 \\ \frac{\rho u}{M^2 P_o} & \frac{u}{2T_o} \left(\rho - \frac{2\rho}{M^2} \right) & -\frac{\rho^2 u^2 v}{\gamma M^2 p} \\ \frac{\rho v}{M^2 P_o} & \frac{v}{2T_o} \left(\rho - \frac{2\rho}{M^2} \right) & \frac{\rho^2 u^3}{\gamma M^2 p} \\ \frac{(\gamma-1)p}{P_o} & \frac{\gamma p}{T} \left[\frac{1}{(\gamma-1)} - \frac{T}{T_o} \right] & 0 \end{pmatrix} \quad (31)$$

where the first line of both operators simply means that δQ_1 is free, in that it represents the effects on the boundary of arbitrary variations in the flow domain.

Therefore, to compute the adjoint inflow sensitivities, one should substitute \mathbf{B}'_α in (26) by (31) for subsonic and by (28) for supersonic flows.

For illustration, Table I shows a summary of the inflow adjoint boundary conditions.

TABLE I
 SUMMARY OF ADJOINT INFLOW BOUNDARY CONDITIONS

Regime	State vector variation	Co-state vector B.C.
subsonic	$\delta Q_2(\delta Q_1), \delta Q_3(\delta Q_1), \delta Q_4(\delta Q_1)$	$\phi_1(\phi_2, \phi_3, \phi_4)$
supersonic	$\delta Q_i = 0$	ϕ_i are free

IV. INCOMPRESSIBLE NAVIER-STOKES FORMULATION

This section is dedicated to construct the adjoint problem for incompressible unsteady Navier-Stokes flows. For that purpose, consider the governing equations:

$$\begin{cases} \partial_o \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + v \nabla p - \nu \nabla^2 \mathbf{u} = 0 \\ \nabla \cdot \mathbf{u} = 0 \end{cases} \quad (32)$$

Then, one can obtain the expression for the augmented functional on imposing the realizability constraints, exactly as it was done in Section III for flows governed by the Euler equations:

$$G = \frac{1}{T} \iint_{0B_w} \mathcal{F} \left| \frac{dS'}{dS} \right| dS dt + \frac{1}{T} \left\{ \int_D \theta \nabla \cdot \mathbf{u} d\chi + \int_\Omega \psi \cdot [\partial_o \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + v \nabla p - \nu \nabla^2 \mathbf{u}] d\Omega \right\} + \frac{1}{T} \iint_{0S_i} \beta (u^i - f^i) dS dt + \langle \mathbf{a}, \alpha - \alpha_o \rangle \quad (33)$$

The measure of merit is usually a functional of the flow variables, as shown in (1). However, body surface integrals are particularly interesting for design applications. Hence one may consider an integral of the dimensionless force the fluid exerts on the body surface, projected onto a given direction \mathbf{e} :

$$\mathcal{F}(\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{e}) = \mathcal{F}^k e_k - p n^k e_k \quad (34)$$

where $\boldsymbol{\sigma}$ is the fluid stress tensor ($\boldsymbol{\sigma} = \boldsymbol{\tau} - p\mathbf{I}$), vector \mathbf{n} represents the unit normal to the body surface, and \mathbf{e} denotes for the direction of projection.

The physical space is represented by (x^i, t) in Cartesian coordinates. The flow domain \mathcal{D} and the time span define the full domain of the problem $\Omega = \mathcal{D} \times (0, T)$.

On computing the first variation of G , one gets:

$$\begin{aligned}
 T\delta G = & \int_{\Omega} \left\{ \varphi^j |_{,j} v \delta p + [\partial_o \varphi_i + u^j \varphi_i |_{,j} - \varphi_j u^j |_{,i} - \Theta |_{,i} + \right. \\
 & + \nu (\varphi_i |_{,j} + \varphi^j |_{,i}) |_{,j} \delta u^i \Big\} d\bar{\xi} dt - \int_{\partial \mathcal{D}} \left\{ [u^j \varphi_i n_j - \Theta n_i + \right. \\
 & + \nu (\varphi_i |_{,j} + \varphi_j |_{,i}) n^j] \delta u^i + v (\delta p n^i - \delta \mathcal{F}^i) \varphi_i \Big\} dS dt + \\
 & - \left[\int_{\mathcal{D}} \varphi_i \delta u^i dV \right]_0^T + \int_{0B_w} \delta \mathcal{F} \left| \frac{dS'}{dS} \right| dS dt + \\
 & + \int_{0B_w} \mathcal{F} \delta \left| \frac{dS'}{dS} \right| dS dt + \int_{\Omega} \frac{\Theta}{J} \left[\delta (J \beta_{q'}^k) u^{q'} \right]_{,k} d\Omega + \\
 & - \int_{\Omega} \frac{\varphi_{r'}}{J} \left\{ \partial_o (\delta J u^{r'}) + \left[\delta (J \beta_{n'}^j) (u^{r'} u^{n'} + \right. \right. \\
 & + \left. \left. g^{r'n'} p v - \nu u_{,p}^{r'} g^{p'n'} \right) \right]_{,j} \Big\} d\Omega + \\
 & + \int_{0S_i}^T \beta \left(\delta u^i - \frac{\partial f^i}{\partial \alpha^k} \delta \alpha^k \right) dS dt + \int_{0S_i}^T \delta \beta (u^i - f^i) dS dt + \\
 & + \langle \mathbf{a}, \delta \alpha \rangle + \langle \delta \mathbf{a}, \alpha - \alpha_o \rangle \quad (35)
 \end{aligned}$$

On driving the first domain integral of (35) to zero for arbitrary physical variations δu and δp , one obtains the incompressible Navier–Stokes adjoint equation:

$$\begin{cases} \varphi^j |_{,j} = 0 \\ \partial_o \varphi_i + u^j \varphi_i |_{,j} - \varphi_j u^j |_{,i} - \Theta |_{,i} + \nu \varphi_i |_{,j} |_{,j} = 0 \end{cases} \quad (36)$$

where φ is the adjoint velocity vector and Θ is the adjoint pressure. The adjoint boundary conditions are obtained by pursuing the same rationale as in Section III, but now with respect to the second and fourth integrals in (35). The third integral in that equation corresponds to the time conditions and it is driven to zero by assuming that $\varphi_{t=T} = 0$. The set of adjoint boundary conditions is given by Table II.

TABLE II
 ADJOINT BOUNDARY CONDITIONS FOR THE INCOMPRESSIBLE
 NAVIER–STOKES EQUATIONS

contour	flow	adjoint
inflow	fixed \mathbf{u}	$\varphi = 0$
outflow	$\frac{\partial \mathbf{u}}{\partial n} = 0$ fixed p	$\frac{\partial \varphi}{\partial n} = -\frac{(\mathbf{u} \cdot \mathbf{n}) \varphi}{\nu}$ $\Theta = 0$
wall	$\mathbf{u} = 0$	$\varphi = -\rho \frac{\partial \mathcal{F}}{\partial \mathcal{F}} \left \frac{dS'}{dS} \right $
sym. plane	$\mathbf{u} \cdot \mathbf{n} = 0$ $\frac{\partial \mathbf{u}^t}{\partial n} = \frac{\partial p}{\partial n} = 0$	$\varphi \cdot \mathbf{n} = 0$ $\frac{\partial \varphi^t}{\partial n} = \frac{\partial \Theta}{\partial n} = 0$

The remaining terms in (35) represent the sensitivity gradient:

$$\begin{aligned}
 T\delta G = & \int_{0B_w}^T \mathcal{F} \delta \left| \frac{dS'}{dS} \right| dS dt + \int_{\Omega} \frac{\Theta}{J} \left[\delta (J \beta_{q'}^k) u^{q'} \right]_{,k} d\Omega + \\
 & - \int_{\Omega} \frac{\varphi_{r'}}{J} \left\{ \partial_o (\delta J u^{r'}) + \left[\delta (J \beta_{n'}^j) (u^{r'} u^{n'} + \right. \right. \\
 & + \left. \left. g^{r'n'} p v - \nu u_{,p}^{r'} g^{p'n'} \right) \right]_{,j} \Big\} d\Omega \\
 & + \int_{0S_i}^T \beta \left(\delta u^i - \frac{\partial f^i}{\partial \alpha^k} \delta \alpha^k \right) dS dt + \langle \mathbf{a}, \delta \alpha \rangle \quad (37)
 \end{aligned}$$

As for control parameters that are not related to flow geometry, they are also imposed as variational constraints on the problem. In essence, boundary condition constraints are imposed by surface integrals, which are not subject to integration by parts. For the sake of space, we refer the reader to [36], [11] for further details on this portion of the derivation. The final expression for the sensitivity gradient reads:

$$\langle \mathbf{a}, \delta \alpha \rangle = \int_{0S_i}^T \left[\nu (\varphi_i |_{,j} + \varphi_j |_{,i}) n^j - \Theta n_i \right] \frac{\partial f^i}{\partial \alpha^k} \delta \alpha^k dS dt \quad (38)$$

V. RESULTS

The results presented in this section correspond to validation test cases for both formulations described in Sections III and IV, where the sensitivity gradients obtained by the proposed approach of the adjoint method are compared with finite differences and theoretical values.

A. Compressible Euler Flow Simulations

The flow and adjoint solutions alike were computed on unstructured meshes with triangular elements. The numerical simulations for both physical and adjoint PDE's have been run with a cell-centered finite volume method, by using 2nd order 5-step Runge–Kutta time-stepping scheme [37] with characteristics-based boundary conditions [34].

The results for compressible Euler are presented for internal and external flows. The former corresponds to flows through a divergent nozzle in both subsonic and supersonic regimes, while the latter corresponds to supersonic flows over a diamond profile. In all compressible test cases, the measure of merit is a pressure integral over the wall surface, which is projected onto the flow normal direction. For simulations over airfoils, it corresponds to the lift force, and it is given by:

$$I_o = \int_{B_w} p \mathbf{n} \cdot \mathbf{e} dS \quad (39)$$

where \mathbf{n} is the normal unit vector pointing into the wall surface and \mathbf{e} is the vertical unit vector, which is normal to the freestream direction.

The dimensionless form of the flow variables is defined on the basis of a reference state, which is the same for all tests in

Section V-A. The reference values are: specific mass, $\rho_{ref} = 1.486 \text{ kg/m}^3$; velocity, $v_{ref} = 320.33 \text{ m/s}$; and temperature, $T_{ref} = 357.77 \text{ K}$.

The computational mesh of the divergent nozzle is shown in Fig. 1. The idea behind the choice of this geometry is to avoid shock waves in the validation procedure.

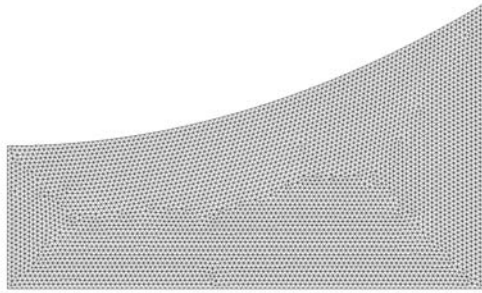


Fig. 1 Divergent nozzle mesh

A comparison between gradients that are obtained by finite differences and the adjoint method is presented in Fig. 2 for subsonic flows with entrance Mach numbers ranging from 0.47 to 0.75. As was mentioned in Section III, inflow angle of incidence, stagnation pressure and temperature are taken as control parameters. Then the gradients obtained are $\partial I/\partial p_o$, $\partial I/\partial T_o$ and $\partial I/\partial \theta$. The differences between both methods remain below 2.9×10^{-3} for all components.

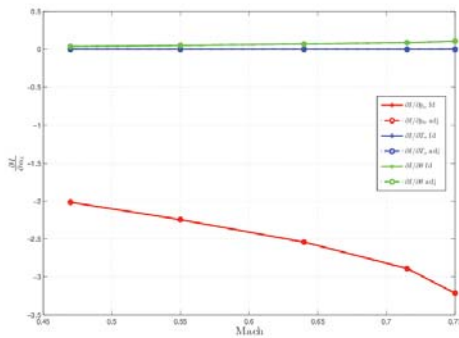


Fig. 2 Gradients of a subsonic flow in a divergent nozzle. Red, $\partial I/\partial p_o$; blue, $\partial I/\partial T_o$; green, $\partial I/\partial \theta$. Solid x, finite difference; dash-dot o, adjoint method

Fig. 3 presents the same comparison for supersonic flows. However, in this case the primitive variables are taken as control parameters. Naturally, the gradients obtained are $\partial I/\partial \rho$, $\partial I/\partial u$, $\partial I/\partial v$ and $\partial I/\partial p$. The simulations were performed for Mach numbers ranging from 1.5 to 2.5. In this case, the differences between both methods remain below 4.6×10^{-4} for all components.

It is interesting to progressively increase the complexity of test cases. Following this idea, the next results correspond to the evaluation of the same sensitivities that are described above, but now for the external flow over a diamond profile. The geometry was chosen so as to have the shock waves

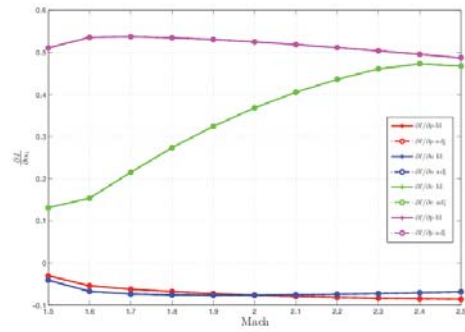


Fig. 3 Gradients of a supersonic flow in a divergent nozzle. Red, $\partial I/\partial \rho$; blue, $\partial I/\partial u$; green, $\partial I/\partial v$; magenta, $\partial I/\partial p$. Solid x, finite difference; dash-dot o, adjoint method

attached to the solid surfaces. In order to illustrate the problem, Fig. 4 shows Mach contours of one test case where the farfield Mach number, $M = 2.0$, and the angle of incidence, $\theta = 4^\circ$.

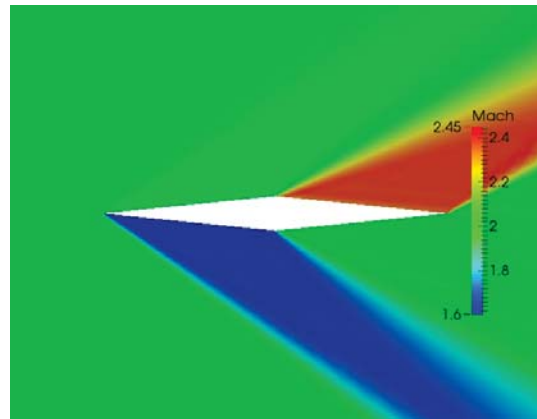


Fig. 4 Mach contour of a diamond profile. Farfield Mach number, $M = 2.0$, and the angle of attack, $\theta = 4^\circ$

The comparison between finite differences and adjoint method gradients is shown in Fig. 5. As it can be seen, the sensitivities are in good agreement for all components of the gradient. In this case, the differences between them remain below 1.7×10^{-2} for all components.

B. Incompressible Navier–Stokes Simulations

Both physical and adjoint simulations were performed by using the code SEMTEX. It is a high order computational code, which has been developed by [38], and which is based on spectral/hp element method.

The test case here consists of a flow through a two dimensional channel. A scheme of the flow is shown in Fig. 6.

The length scale for the channel flow is the hydraulic diameter (D_h):

$$D_h = 2.H \quad (40)$$

The computational mesh for flow and adjoint simulations is shown below. It was generated with *Gambit* and has 1020 quadrilateral elements.

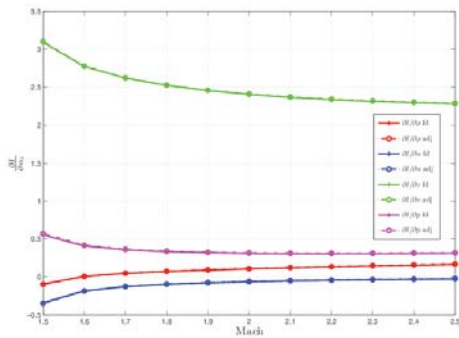


Fig. 5 Sensitivity gradients of the lift with respect to the primitive variables in a supersonic flow over a diamond profile with angle of attack, $\theta = 4^\circ$. Red, $\partial I/\partial \rho$; blue, $\partial I/\partial u$; green, $\partial I/\partial v$; magenta, $\partial I/\partial p$. Solid x, finite difference; dash-dot o, adjoint method

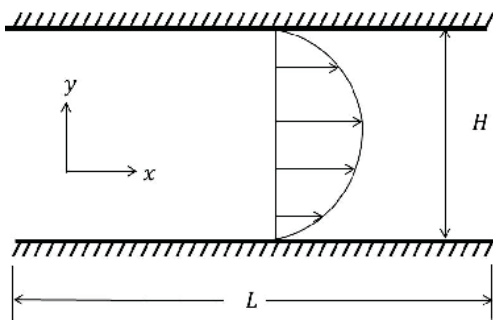


Fig. 6 Flow through a 2-D channel between two flat plates separated by a distance of H and with length L

The mesh is defined in $-1 \leq x \leq 100$. For visualization purposes it is shown only the region near the inflow boundary. Fig. 8 shows both flow and adjoint solutions. The simulation parameters are $Re = 30$, polynomial order $P = 10$ and 40000 time steps, each one with magnitude $\Delta t = 10^{-3}$.

The analytical expression for the gradient $\frac{dC_d}{dU_\infty}$ is:

$$\frac{dC_d}{dU_\infty} = -\frac{48}{U_\infty Re} \quad (41)$$

The sensitivity gradient expression for this specific case is:

$$\frac{dC_d}{dU_\infty} = \frac{1}{Re} \int_{\tilde{S}_i} \{[\nabla \varphi + (\nabla \varphi)^T] - \Theta \mathbf{I}\} \mathbf{n} d\tilde{S} \quad (42)$$

Simulations are taken for different values of Re and, for each one, the gradient is computed. The results are shown on Fig. 7.

The red curve corresponds to the analytical expression whereas the blue circles represent the adjoint gradients. It is possible to see that the adjoint gradients are quite close to the analytical ones (error less than 1%), proving that it is possible to compute a non-geometric sensitivity using the adjoint method.

VI. CONCLUSION

The main objective of this paper has been to illustrate a novel approach to computing non-geometric sensitivities with the adjoint method. It makes use of the same adjoint solution

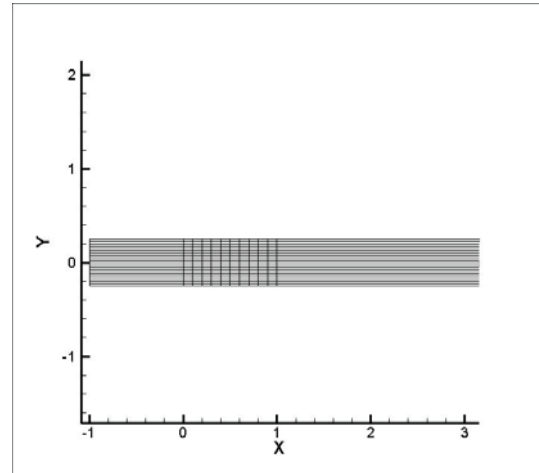
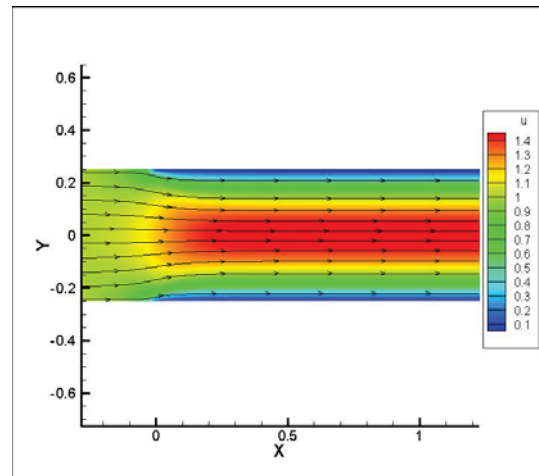
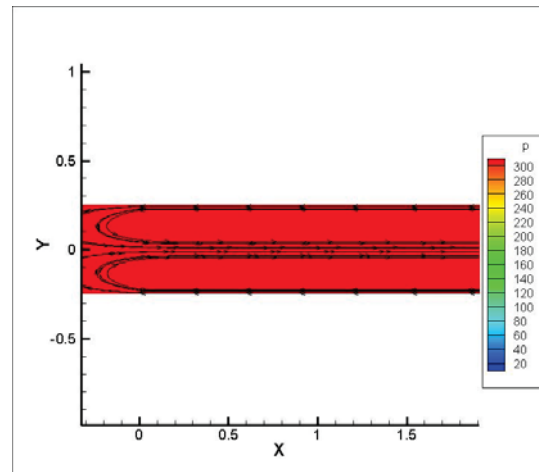


Fig. 7 Computational mesh for the 2-D flow



(a) Flow solution with streamtraces and contours of horizontal velocity u



(b) Adjoint solution with streamtraces and contours of adjoint pressure Θ

Fig. 8 Flow through a 2-D channel. Details for flow and adjoint solutions

that is used for geometry optimisation. The 2-D flows have been chosen for this purpose, for their simplicity. However,

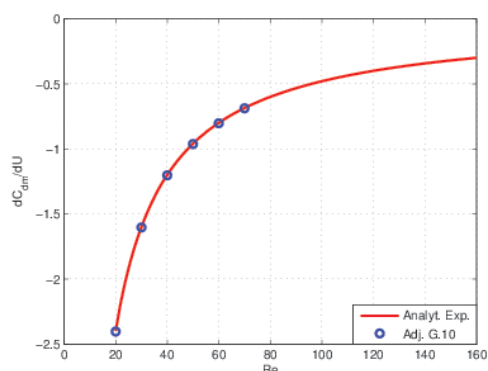


Fig. 9 Sensitivity gradient dC_d/dU_∞ . Red line, analytical expression; blue circles, adjoint method

from the theoretical point of view, the same approach can be applied to 3-D flows just as well. Moreover, it has been shown that these findings can be applied to internal and external flows alike, in both subsonic and supersonic regimes, as well as for viscous incompressible flows. The results for supersonic flows with shock waves show less accuracy, when compared to the others. To tackle that problem, we are currently investigating the effects of mesh refinement and shock smearing, and we have gotten some encouraging results, albeit preliminary.

Although still limited in scope, the above results open up some interesting possibilities of further research. First and foremost the extension to 3-D flows, which is merely algebraic, would allow one to use this approach to evaluate stability derivatives, for flight dynamics applications. The idea of extending the approach to compressible viscous flows is certainly attractive, but it is further down the road. Time dependent flows are also a promising subject. In effect, the formulations for incompressible viscous is already compatible with transient flows, and we are working on it.

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