A SYSTEMATIC FORMULATION OF THE CONTINUOUS ADJOINT METHOD APPLIED TO VISCOUS AERODYNAMIC DESIGN

A Systematic Formulation of the Continuous Adjoint Method Applied to Viscous Aerodynamic Design

C. Castro*, C. Lozano†, F. Palacios‡ and E. Zuazua‡

*Departamento de Matemáticas e Informática, ETSI Caminos, Canales y Puertos.
Universidad Politécnica de Madrid, Madrid, 28040, Spain
E-mail: carlos.castro@upm.es

†Área de Dinámica de Fluidos, Departamento de Aerodinámica y Propulsión.
Instituto Nacional de Técnica Aeroespacial, Torrejón de Ardoz, Madrid, 28850, Spain
E-mail: lozanorc@inta.es

‡IMDEA Matemáticas
Facultad de Ciencias, UAM, Campus de Cantoblanco, Madrid, 28049, Spain
E-mail: francisco.palacios@imdea.org, enrique.zuazua@uam.es

Key Words: aerodynamic design optimization, continuous adjoint method

ABSTRACT

A continuous adjoint approach to aerodynamic design for viscous compressible flows on unstructured grids is developed, and three important problems raised in the continuous adjoint literature are solved: using tools of shape deformation of boundary integrals a generic adjoint formulation is developed with independence of the kind of mesh used; a systematic way of reducing the 2nd order derivative terms which arise is presented which avoids the need of using higher order numerical solvers to obtain accurate approximations of the 2nd order derivatives; and finally, the class of admissible optimization functionals is clarified. Several remarks are made concerning the longstanding discrete vs. continuous adjoint dichotomy, with the emphasis not on the advantages or disadvantages of each method, but rather on the well-posedness of the approaches. The accuracy of the sensitivity derivatives is assessed by comparison with finite-difference computations, and the validity of the overall methodology is illustrated with design examples under demanding subsonic conditions.

I. INTRODUCTION

Aerodynamic design optimization by adjoint methods (control theory) has received much attention recently since the pioneering work of Jameson[1,2]. In these methods the goal is to evaluate the response (sensitivity derivatives or gradients) of a given functional of the flow to a change of defining parameters (control or design variables): surface deformations, change in angle of attack or Mach number, etc. These gradients are then used as input for an appropriate optimization module[3].

The fundamentals of the procedure are as follows. We restrict ourselves to shape-deformation problems. Classical aeronautical applications of optimal shape design in systems governed by PDEs consider a fluid domain Ω (usually air) delimited by disconnected boundaries divided into a “far field” Γ_∞ and several solid wall boundaries S (usually airfoil or airplane surfaces).

This kind of design problems is aimed at minimizing a functional J of the flow that has been defined on the boundaries S, Γ_∞, or in a subdomain $\omega \subset \Omega$. From now on we will restrict ourselves to the analysis of optimization problems involving functionals defined on the solid wall S, whose value depends on the flow variables U obtained from the solution of the corresponding fluid flow equations (Euler or Navier-Stokes equations). In this context, the generic optimization problem can be succinctly stated as follows

$$J(S^{\min}) = \min_{S \in \mathbf{S}_{ad}} J(S)$$

where $S^{\min}$ is the seeked optimal surface (belonging to the set $\mathbf{S}_{ad}$ of admissible boundary geometries) and

$$J = \int_S g\left(U, \vec{n}\right) ds,$$

is the objective or cost function, whose evaluation is subject to the resolution of the flow equations. Here *g* is a given smooth function, *U* are the flow variables, subject to the (steady) flow equations (2D or 3D Euler or Navier-Stokes equations), and $\vec{n}$ is the outward unitary normal vector to *S*.

In practical applications, a numerical discretization in space and time is needed to evaluate the functional *J*, as well as the flow variables *U*. Generically, the continuous problem is replaced by the following discrete problem: find $S_h^{\min}$ (within the set of admissible discrete boundary geometries $\mathbf{S}_{h\,ad}$) for which

$$J_h(S_h^{\min}) = \min_{S_h \in \mathbf{S}_{had}} J_h(S_h)$$

where *h* represents a characteristic length of the spatial discretization. Thus, in practice, one has to optimize a finite dimensional system coming from a suitable discrete numerical approximation scheme of PDEs. An efficient optimization process can be implemented using a gradient method and the most natural way to obtain the gradients of the objective function would appear to be the adjoint method. This method requires the computation of the solution of the adjoint to the linearized discrete flow equations. This method is usually referred as *discrete adjoint method*. Nevertheless, the use of this methodology requires making certain assumptions concerning the differentiability of the numerical schemes used, which are not generally verified, because the best suited (and most popular) methods for the resolution of the Euler equations (Roe[4], JST[5], etc) are non-differentiable. To make things work in practice, several alternatives have been proposed, such as to freeze the non-differentiable terms of central schemes with high-order artificial viscosity when using the discrete adjoint approximation[6], to develop pseudo-linearized models for Godunov schemes, and to use the continuous approach as a shortcut[7,8], keeping in mind that the goal is to minimize a discrete functional and that the comparison of “gradients” of different functionals, or of different discrete representations of the same continuous functional, may be a delicate issue, as very different functionals may have very close minima, their gradients being significantly different.

An alternative to the dicrete adjoint method is the *continuous adjoint methodology*. Here, the main idea is to come back to the continuous formulation of the problem and derive the adjoint problem from the flow equations. This makes it possible to obtain a gradient for the continuous functional *J*, and a suitable discretization of this gradient can be used as a descent direction for the discrete functional. It is worth mentioning that this procedure is far from being justified from a mathematical point of view, in general.

In this work we focus on the first part of this continuous adjoint methodology, namely the computation of the gradient of the continuous functional. We present a generic adjoint formulation which clarifies some of the main drawbacks to the continuous adjoint method present in the literature. More precisely, we use tools of shape deformation of boundary integrals to obtain a generic adjoint formulation with independence of the kind of mesh used, which is suitable for any admissible functional. This formulation makes appear 2nd order derivatives of the flow variables at the boundary. This requires costly higher order numerical solvers to obtain accurate approximations. To overcome this difficulty we reduce the order of these derivatives by writing the flow equations on the boundary in local coordinates. In this way, normal derivatives can be written as tangential ones that can be reduced by integration by parts.

A fundamental problem present in our analysis, and which is not addressed here, is the possible presence of discontinuities in the solutions of the flow equations. In this case, shocks must be treated as singularities and the Rankine-Hugoniot conditions must be included. To obtain the adjoint system, a suitable linearization of these adjoint Rankine-Hugoniot conditions must be accomplished. The new formulation is the object of forthcoming works (see[9] for some numerical preliminary results). Recently, several authors have proposed a procedure to obtain the adjoint-based gradient of these cost functionals without introducing the adjoint variables for the shock position[10].

II. OVERVIEW OF CONTINUOUS ADJOINT FORMULATION

Given a control boundary surface *S*, we consider a generic deformation defined as a vector field $\delta\vec{x}$ on *S*. In general, $\delta\vec{x}$ is assumed to belong to a finite dimensional space generated by a suitable set of basis functions. Deforming the boundary *S* induces a perturbation in the flow, which can be characterized, for small deformations, by the solution δU of the linearized flow equations, which are spelled out in detail below. As both *S* and the flow have changed, the functional *J* varies, too, and the corresponding variation can be generically written as follows

$$\delta J = \underbrace{\int_{\delta S} g\left(U,\vec{n}\right)ds}_{\text{Geometric variation}} + \underbrace{\int_{S} \frac{\partial g}{\partial U}\delta U ds}_{\text{Flow variation}}.$$

The geometric variation part contains three terms[7,11]

$$\int_{\delta S} g\left(U,\vec{n}\right)ds = \underbrace{\int_{S} \frac{\partial g}{\partial U}\left(\delta\vec{x}\cdot\vec{\nabla}U\right)ds}_{\text{Displacement Term}} + \underbrace{\int_{S}\left(\frac{\partial g}{\partial \vec{n}}\delta\vec{n}\right)ds}_{\text{Variation of the normal}} + \underbrace{\int_{S} g\delta ds}_{\text{Curvature Term}}$$

where the curvature term has the form

$$\int_{S} g\delta ds = \int_{S} g\mathrm{K}ds, \quad \mathrm{K} = \begin{cases} \left(\partial_{tg}\delta x_t - \kappa\delta x_n\right) & \text{(2D)}, \quad \kappa \quad \text{curvature of profile} \\ \left(\vec{\nabla}_{tg}\cdot\delta\vec{x}_t - 2\mathrm{H}_m\delta x_n\right) & \text{(3D)}, \quad \mathrm{H}_m \quad \text{mean curvature of surface} \end{cases}$$

where $\delta x_n = \delta\vec{x}\cdot\vec{n}$ (resp. $\delta\vec{x}_t = \delta\vec{x} - \delta x_n\vec{n}$) is the normal (resp. tangent) part of the surface deformation.

As for the flow variation term, its form depends on the cost function under consideration, but it contains, in general, variations of flow variables such as the pressure δP or the viscous stresses $\delta\sigma_{ij}$ which can only be computed by solving, for any vector field $\delta\vec{x}$ describing the surface deformation, the linearized flow equations

$$\vec{\nabla}\cdot\left(\left(\vec{A}+\vec{A}^{v}\right)^{T}\delta U\right) - \frac{\partial}{\partial x^{i}}\left(\left[D_{ij}\frac{\partial\delta U}{\partial x^{j}}\right]\right) = 0$$

$$\vec{A} = \left(\partial\vec{F}/\partial U\right)^{T}, \quad \vec{A}^{v} = -\left(\partial\vec{F}^{v}/\partial U\right)^{T}, \quad D_{ij} = \left(\partial F^{v}{}_{i}/\partial\left(\partial U/\partial x^{j}\right)\right)^{T}$$

(summation over repeated indices $i, j = 1,\ldots,3$ is understood) and linearized boundary conditions

$$\left.\delta\vec{u}\right|_{S} = -\delta x_i\partial_i\vec{u}$$

$$\left.\partial_n\delta T\right|_{S} = -\delta\vec{n}\cdot\vec{\nabla}T - n_i\delta x_j\partial_j\partial_i T$$

on *S* (where $\vec{u}$ is the flow velocity vector, *T* is the fluid temperature and an adiabatic thermal boundary condition has been assumed), as well as linearized characteristic boundary conditions on Γ_{∞}. This procedure is computationally prohibitive when the dimension of the space of design variables $\delta\vec{x}$ (i.e., the number of independent surface deformations considered) is large, so the standard procedure is to introduce the adjoint state Ψ subject to the adjoint equations:

$$\left(\vec{A}+\vec{A}^{v}\right)\cdot\vec{\nabla}\Psi^{T}+\frac{\partial}{\partial x^{i}}\left(\left[D_{ji}\frac{\partial\Psi^{T}}{\partial x^{j}}\right]\right)=0$$

where $\vec{F}$ and $\vec{F}^{v}$ are the inviscid and viscous flux vectors, respectively, along with the appropriate adjoint boundary conditions on S so as to allow the computation of the flow variation term[1,2,7,11]. The resulting expressions are suitable for optimization under viscous as well as inviscid flow equations. The procedure also allows the determination of the general structure of the functionals. For functionals defined on a control surface S and subject to the Navier-Stokes equations with non-slip and adiabatic boundary conditions the structure of the admissible functional is the following

$$\int_{S} g\left(\vec{f},T\right)ds,\quad \vec{f}=P\vec{n}-\vec{n}\cdot\sigma\,.$$

The corresponding adjoint boundary conditions on S are

$$\left(\psi_{2},\psi_{3},\psi_{4}\right)=\left(\frac{\partial g}{\partial f_{x}},\frac{\partial g}{\partial f_{y}},\frac{\partial g}{\partial f_{z}}\right),$$
$$k\partial_{n}\psi_{5}=\frac{\partial g}{\partial T}$$

where $\left(\psi_{1},\ldots,\psi_{5}\right)$ are the components of the adjoint state and k is the coefficient of thermal conductivity. Therefore, optimization is possible in this case with respect to any of the components of the total force $\vec{f}$ exerted by the fluid on the wall (including both the pressure and the viscous stress terms), as well as with respect to surface temperature distributions T. In particular, functions that depend solely on the pressure are allowed, by considering $g\left(\vec{f},T\right)=\vec{n}\cdot\vec{f}$ since $\vec{n}\cdot\sigma\cdot\vec{n}=0$ on S. This possibility has been largely ignored in the literature.

We now focus on the case of total drag minimization, for which the cost function is

$$J=\int_{S}\left(\vec{f}^{*}\cdot\vec{d}\right)ds,\quad \vec{f}^{*}=C_{p}\vec{n}-\frac{1}{C_{\infty}}\vec{n}\cdot\sigma,$$

where $C_{p}=\left(P-P_{\infty}\right)/C_{\infty}$ is the non-dimensional pressure coefficient, $C_{\infty}=\gamma M_{\infty}^{2}P_{\infty}/2$ is the reference dynamic pressure, γ is the adiabatic exponent (or ratio of specific heats of the fluid), P_{∞} and M_{∞} are the free-stream Pressure and Mach number, and $\vec{d}$ is a constant vector directed along the flow direction. The variation of this cost function is

$$\delta J=\int_{S}\left(\frac{1}{C_{\infty}}\left((\delta\vec{x}\cdot\vec{\nabla}P)(\vec{n}\cdot\vec{d})-n_{i}d_{j}\delta\vec{x}\cdot\vec{\nabla}\sigma_{ij}\right)+\mathrm{K}\left(\vec{f}^{*}\cdot\vec{d}\right)+\delta\vec{n}\cdot\left(C_{p}\vec{d}-\frac{1}{C_{\infty}}\sigma\cdot\vec{d}\right)\right)ds$$
$$-\int_{S}\left((\vec{n}\cdot\delta\vec{u})\left(\rho\psi_{1}+\rho H\psi_{5}\right)-\psi_{5}\vec{n}\cdot\sigma\cdot\delta\vec{u}+\vec{n}\cdot\Sigma\cdot\delta\vec{u}-k\psi_{5}\partial_{n}\delta T\right)ds$$

where ρ is the density of the fluid, H is the enthalpy and $\Sigma_{ij} = \mu\left(\frac{\partial\psi_{i+1}}{\partial x_j} + \frac{\partial\psi_{j+1}}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial\psi_{k+1}}{\partial x_k}\right)$ is the adjoint stress tensor. The computation of the above expression requires the specification of the following linearized and adjoint boundary conditions on S

$$
\begin{gathered}
\delta\vec{u}\big|_S = -\delta x_i \partial_i \vec{u}, \\
\partial_n \delta T\big|_S = -\delta\vec{n}\cdot\vec{\nabla}T - n_i \delta x_j \partial_j \partial_i T \\
\left(\psi_2,\psi_3,\psi_4\right)\big|_S = \frac{1}{C_\infty}\left(d_x, d_y, d_z\right), \\
\partial_n \psi_5\big|_S = 0,
\end{gathered}
$$

as well as appropriate boundary conditions on Γ_∞. It can be observed from the previous results that in the variation of the above functional, and in general in the computation of sensitivity derivatives for viscous flows, second order derivatives of the flow variables on S are required (such as those appearing in $\vec{\nabla}\sigma_{ij}$ and $\partial_n \delta T$). This is cumbersome (and has in fact been pointed out as a drawback of the approach[11]) as the accurate numerical evaluation of such derivatives requires at least third-order spatial accuracy, which is beyond the capabilities of most unstructured flow solvers. This issue has been solved with the development of a systematic way of reducing the order of the higher derivative terms[7] which amounts to the use of the flow equations restricted to S to convert the normal derivatives on the second order terms into tangent derivatives and integrate those by parts to reduce the order of the derivatives. Pick for example the term $\partial_n \delta T\big|_S$, which according to the thermal boundary condition is equal to $-\delta\vec{n}\cdot\vec{\nabla}T - n_i\delta x_j \partial_j \partial_i T$. The corresponding terms in the variation can be reduced as follows (the details can be found in[7])

$$
\int_S k\psi_5 n_i \delta x_j \left(\partial_i \partial_j T\right) ds + \int_S k\psi_5 \left(\delta\vec{n}\cdot\vec{\nabla}T\right) ds = \int_S \delta x_n k\psi_5 \left(\partial_n{}^2 T\right) ds - \int_S k\psi_5 \left(\vec{\nabla}_{tg}\delta x_n\right)\cdot\left(\vec{\nabla}_{tg}T\right) ds
$$

where $\vec{\nabla}_{tg}$ is the tangent derivative on the surface. The term containing two normal derivatives can be rewritten as follows

$$
k\partial_n{}^2 T\big|_S = \vec{\nabla}\cdot\left(k\vec{\nabla}T\right)\Big|_S - \vec{\nabla}_{tg}\cdot\left(k\vec{\nabla}_{tg}T\right) = -\sigma_{ij}\partial_i u_j - \vec{\nabla}_{tg}\cdot\left(k\vec{\nabla}_{tg}T\right)
$$

after using the energy flow equation on S,

$$
\vec{\nabla}\cdot\left(k\vec{\nabla}T\right)\Big|_S = -\sigma_{ij}\partial_i u_j\big|_S
$$

The net result is

$$
\int_S k\psi_5 n_i \delta x_j \left(\partial_i \partial_j T\right) ds + \int_S k\psi_5 \left(\delta\vec{n}\cdot\vec{\nabla}T\right) ds = -\int_S \delta x_n \psi_5 \sigma_{ij}\partial_i u_j ds + \int_S \delta x_n k\left(\vec{\nabla}_{tg}\psi_5\right)\cdot\left(\vec{\nabla}_{tg}T\right) ds
$$

which only contains first derivatives of the flow variables. Other second-order terms can be treated in a similar fashion. With this strategy, more compact expressions result that can be evaluated with second-order accurate flow solvers. For, e.g., drag minimization, the following expression is obtained[7]:

$$\delta J = \int_S \delta x_n G ds,$$

where G, which is the local sensitivity, is the following computable function of the flow and adjoint variables and their first derivatives

$$G = (\vec{n}\cdot\partial_n\vec{u})\left(\rho\psi_1+\rho H\psi_5\right)+\vec{n}\cdot\Sigma\cdot\partial_n\vec{u}-\psi_5\left(\vec{n}\cdot\sigma\cdot\partial_n\vec{u}\right)+\psi_5\left(\sigma_{ij}\partial_i u_j\right)-k\left(\vec{\nabla}_{tg}\psi_5\right)\cdot\left(\vec{\nabla}_{tg}T\right).$$

Therefore, sensitivities do not depend on the tangent part of the deformation of the control surface, and the local sensitivity G, which by definition is the direction of optimal deformation, can be used as deformation function (instead of conventional Hicks-Henne functions, for example).

III. NUMERICAL RESULTS AND CONCLUSIONS

As an example of the overall developments, Figs. 1 and 2 show a viscous design example carried out with the methodology described in this work. The proposed design problem starts with a NACA0012 airfoil at a Mach number of 0.3, angle of attack of 2.50º and low Reynolds number of 1000 to keep the flow laminar along the airfoil. The objective is drag minimization by modifying the shape of the airfoil, increasing the lift to 0.15 and using 3 geometrical constraints: minimum value for the greatest thickness (12%), frozen curvature at the leading edge and minimum thickness at 75% of the chord.

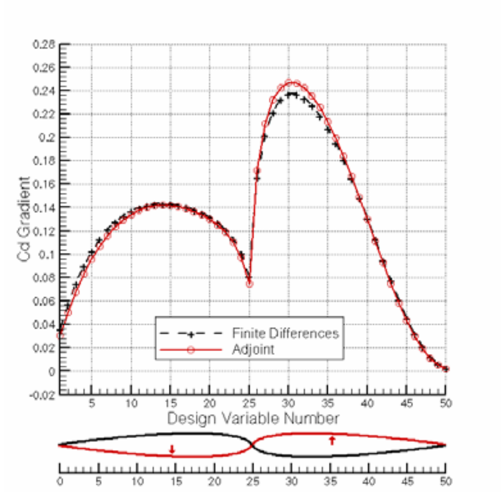

Fig. 1. Viscous C_d subsonic gradients

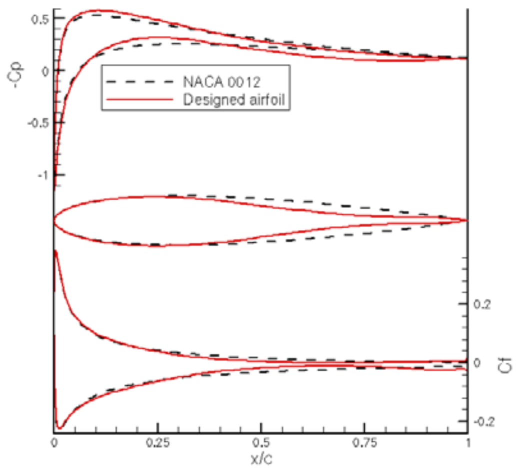

Fig. 2. Initial and designed C_p and C_f

In Fig. 1 a comparison between the gradients computed by finite-difference and adjoint methods is shown. The agreement is excellent. The results of the subsonic optimization are shown in Fig. 2. After 9 design cycles the new airfoil based on a NACA0012 has a drag of 0.1225 that is a 97% of the original NACA 0012 drag (reduction of 36 counts), while the final lift is a 111% greater than the original one.

To sum up, a systematic continuous adjoint approach to aerodynamic design optimization has been presented in this work. The resulting expressions are suitable for optimization under viscous as well as inviscid flow conditions on unstructured as well as structured grids. Some crucial problems are solved and new points of view and investigation lines are proposed in this work.

The results presented here are promising, but further numerical tests are necessary. In particular, a detailed study of the influence of the mesh sensitivities on the formulation, and of a possible strategy for incorporating them, should be carried out. Also, work to extend the methodology to deal with general turbulent three-dimensional flows, and more careful analysis concerning transonic flows, must be undertaken.

REFERENCES

[1]Jameson, A., "Aerodynamic Design Via Control Theory," *Journal of Scientific Computing*, Vol. 3, 1988, pp. 233–260.

[2]Jameson, A., "Optimum Aerodynamic Design Using CFD And Control Theory," *AIAA Paper 95–1729*, 1995.

[3]Monge, F. and Palacios, F., "Inviscid Multipoint Airfoil Optimisation Using Control Theory," *ERCOFTAC Design Optimisation: Methods & Applications. International Conference & Advanced Course Program*, Athens (Greece), 2004.

[4]Roe, P., "Approximate riemann solvers, parameter vectors, and difference schemes," *Journal of Computational Physics*, Vol. 135, 1997, pp. 250–258.

[5]Jameson, A., Schmidt, W., and Turkel, E., "Numerical solution of the euler equations by finite volume methods using runge-kutta time stepping schemes," *AIAA Paper*, Vol. 81, 1981, pp. 1259.

[6]Nadarajah, S., and Jameson, A., "A Comparison of the Continuous and Discrete Adjoint Approach to Automatic Aerodynamic Optimization," AIAA paper 2000–0667, *38th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, NV, January 2000.

[7]Castro, C., Lozano, C., Palacios, F., and Zuazua, E., "Systematic Continuous Adjoint Approach to Viscous Aerodynamic Design on Unstructured Grids," *AIAA Journal*, Vol. 45, No. 9, September 2007, pp. 2125–2139.

[8]Jameson, A., Sriram, S., and Martinelli, L., "A continuous adjoint method for unstructured grids," *AIAA Paper 2003-3955*, 2003.

[9]Giles, M. and Pierce, N., "Analytic adjoint solutions for the quasione-dimensional Euler equations," *J. Fluid Mechanics*, Vol. 426, 2001, pp. 327–345.

[10]Ulbrich, S., "Adjoint-based derivative computations for the optimal control of discontinuous solutions of hyperbolic conservation laws," *Systems and Control Letters*, Vol. 48, 2003, pp. 313–328.

[11]Anderson, W. K. and Venkatakrishnan, V., "Aerodynamic Design Optimization on Unstructured Grids with a Continuous Adjoint Formulation," *Computers and Fluids*, Vol. 28, 1999, pp. 443–480.