Adjoint Techniques for Aerodynamic Shape Optimization Problems: New Mathematical Formulations and Software Assessment for Well–Posed Problems with Acceptable Solutions

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1 Scope of the Project–Summary

Nowadays, a great interest exists upon the development of fast and reliable design and optimization tools for use, among other, in aerodynamic shape inverse design or optimization problems. According to the relevant literature, research focuses on both gradient-based (deterministic) and evolutionary algorithms, or even their hybridization. Gradient-based design methods utilize descent algorithms (practically, steepest descent) supported by tools that compute the gradient of the objective function. For the latter, the adjoint method, basically inspired by control theory concepts, undertakes the gradient computation through the numerical solution of the co-state problem, i.e. the so-called adjoint equations. Henceforth, as it usually occurs in the relevant literature, the term "adjoint method" will be used to denote either the technique (mathematical formulation and software) used to compute the gradient of a functional or the full optimization (minimization) algorithm, the most important part of which is the solution of the co-state problem.

In fluid mechanics, aerodynamics or turbomachinery, a shape optimization problem is related to the design of airfoils, wings or compressor-turbine blades, with either prescribed or optimal performance. Indicative examples of functionals utilized in aerodynamic design are: lift maximization, drag minimization, control of flow separation, heat transfer or transition to turbulence etc. A particular class of design problems, which are usually referred to as inverse design problems, make use of a prescribed pressure or velocity or any boundary layer quantity distribution along the shape contour and seek for the shape that reproduces this distribution at given flow conditions.

The comparison between adjoint methods and evolutionary algorithms as design tools is known; however, it is presented herein in brief, in order to provide reasoning for this research. The adjoint method requires a considerable investment for its development (formulation, programming of software and testing); once this is done, adjoint methods coupled with a simple descent algorithm can locate optimal solutions in the expense of a few only function evaluations, i.e. with reasonable CPU cost. An additional advantage is that this cost does not depend upon the number of design variables. However, the final solution depends on the initialization, so the adjoint method is likely to be trapped into local minima. On the other hand, evolutionary algorithms bear negligible development cost, accommodate readily any "external" evaluation software but, despite their robustness, require a great amount of function evaluations to reach the optimal solution; the cost increases with the number of design variables.

The development of accurate adjoint formulations, for "any" objective function, is a complex "oriented basic research" issue.

This Basic Research Project is entitled "*Adjoint Techniques for Aerodynamic Shape Optimization Problems: New Mathematical Formulations and Software Assessment for Well-Posed Problems with Acceptable Solutions*", and focuses only on the adjoint method as an optimization tool. It tackles the problem of non-well-posed functionals: quite often, though the design target is "simple" at first glance (such as: compute an aerodynamic shape with a prescribed velocity distribution over its contour), the corresponding functional leads to non-well-posed adjoint formulations. To overcome this problem, attention should be paid to the mathematical formulation leading to the adjoint equations and their boundary conditions. This is where this project is focusing on.

Two approaches related to the formulation of the adjoint equations exist: *the continuous adjoint method*, in which the adjoint equations are first derived from the flow partial differential equations (pdes) and then discretized and the *discrete* one, in which the discrete adjoint equations are derived from the discretized flow equations. This project deals with the continuous adjoint method (in the sense that the software developed is based on the latter) but all outcomes can also be transferred to discrete adjoint formulations in a straightforward manner.

During the first phase of the project, we worked on the establishment of the mathematical framework for continuous adjoint formulations. The corresponding software was programmed and tested in a number of test cases. Then, we reformulated the problem in order to account for problems in which the conventional formulation leads to non-well-posed problems.

2 $1D$ Adjoint Formulation

In order to create a solid basis for this research, we started by working on a quasi–1D flow problem in a hypothetical duct. The compressible flow is developed along the x direction. $S(x)$ is the cross section variation along this direction. Mathematically, there is an important difference between this case and the $2D$ or $3D$ cases which follow. In the quasi–1D problem, the target is a flow variable distribution along the hypothetical duct axis, i.e. along which the the flow equations are solved, too. In contrast, the $2D$ and $3D$ flows require the formulation of field flow and adjoint problems and the target is defined only along a part of the boundary.

The objective functional

$$F(\vec{U},\vec{b}) = \frac{1}{2}\int_{(L)} (p(x) - p_{tar}(x))^2 dx \tag{1}$$

reflects the deviation from a desired pressure distribution along the axis. Its variation is augmented with the variation of the flow equations, multiplied by the adjoint variables and integrated along the duct. The flow equations in quasi–1D flows are written as

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{f}}{\partial x} = \vec{q} \tag{2}$$

where $\vec{U} = [\rho\ \rho u\ \rho E]^T$ is the conservative variable vector, $\vec{f} = \left[\rho u \quad \rho u^2 + p \quad u\,(\rho E + p)\right]^T$, the inviscid flux vector and $\vec{q} = -\frac{1}{S}\frac{dS}{dx}\left[\rho u \quad \rho u^2 \quad u\,(\rho E + p)\right]^T$ the source term. So, the variation of the augmented objective functional reads

$$\delta F_{aug} = \delta F - \int_L \vec{\Psi}^T \left(\frac{\partial \delta \vec{f}}{\partial x} - \delta \vec{q} \right) dx \tag{3}$$

After some mathematical calculations, the variation is finally written as

$$\begin{aligned}
\delta F_{aug} = & \underbrace{\int_{(L)} \delta \vec{U}^T \left[(p - p_{tar})(\frac{\partial p}{\partial \vec{U}})^T + A^T \frac{\partial \vec{\Psi}}{\partial x} + T^T \vec{\Psi} \right] dx}_{A.E.} \\
& - \underbrace{\left[\vec{\Psi}^T A \delta \vec{U} \right]_{out} + \left[\vec{\Psi}^T A \delta \vec{U} \right]_{in}}_{A.E.B.C.} \\
& + \tfrac{1}{2} \underbrace{\int_{(L)} (p - p_{tar})^2 \delta dx + \int_L \vec{\Psi}^T R \delta \vec{b}\, dx}_{S.D.}
\end{aligned} \tag{4}$$

The terms marked with $A.E.$ give the field adjoint equations

$$\frac{\partial \overrightarrow{\Psi}}{\partial t} - \left(A^T \frac{\partial \overrightarrow{\Psi}}{\partial x} + T^T \overrightarrow{\Psi} + (p - p_{tar})(\frac{\partial p}{\partial \overrightarrow{U}})^T \right) \; = \; 0 \tag{5}$$

Those terms marked with $A.E.B.C.$ are eliminated by imposing the adjoint boundary conditions

$$\delta \overrightarrow{U}^T A^T \overrightarrow{\Psi} \; = \; 0 \tag{6}$$

and, finally, terms marked with $S.D.$ give the sensitivity derivative expression

$$\frac{\delta F}{\delta b_i} \; = \; \int_L \overrightarrow{\Psi}^T \overrightarrow{R}_i dx \tag{7}$$

where

$$\overrightarrow{R}_i = \frac{\delta \overrightarrow{q}}{\delta b_i} = \frac{\delta(-\frac{1}{S}\frac{\partial S}{\partial x})}{\delta b_i} \begin{bmatrix} \rho u & \rho u^2 & u(\rho E + p) \end{bmatrix}^T \tag{8}$$

Before employing eq. 8, the parameterization technique method should be defined. Other flow variables can be set as target as well, leading to different adjoint equations and sensitivity derivatives. The major problem is whether the new formulations lead to well–posed problems.

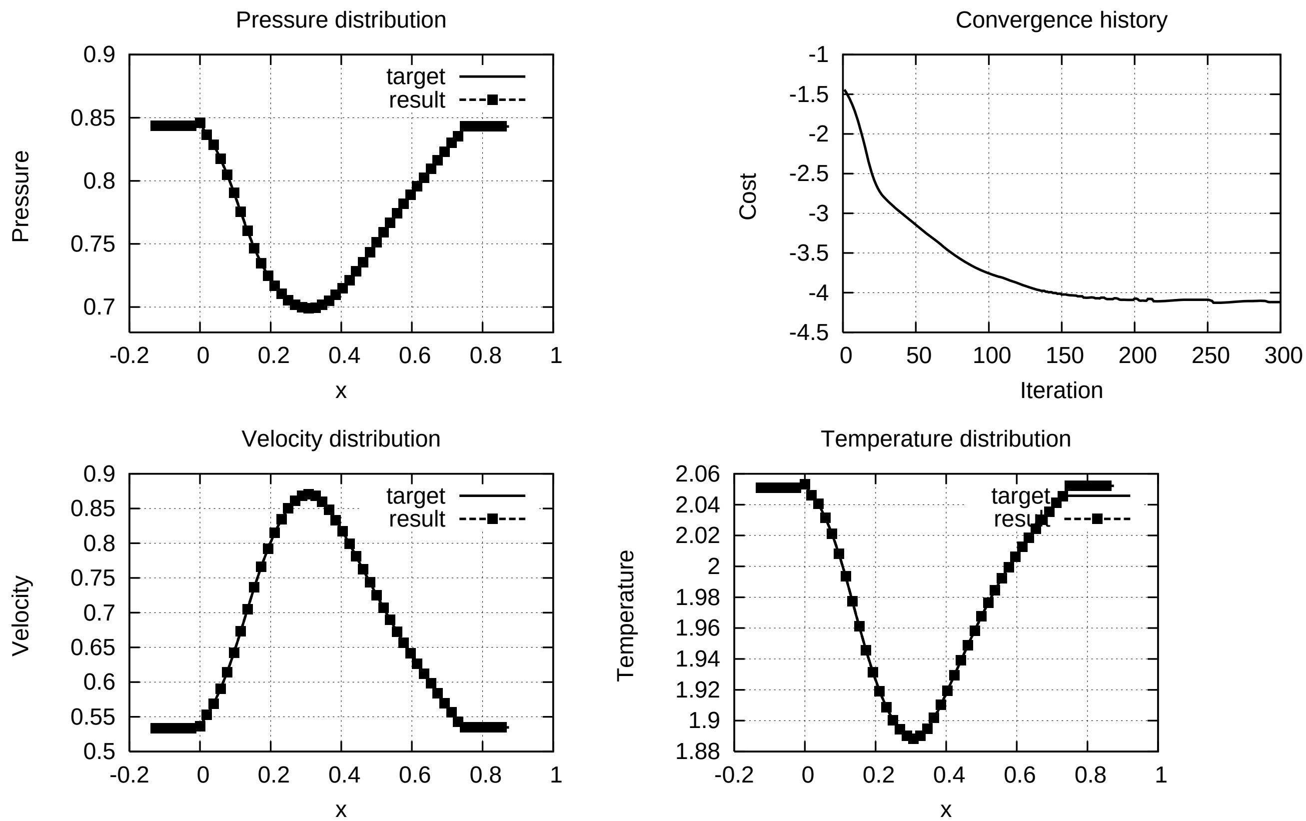

Figure 1: Quasi–1D inverse design with the target being a desired pressure (top–left), velocity (bottom–left) and temperature (bottom–right) distribution. The convergence of the steepest descent algorithm is also shown (top–right).

Once the adjoint method has been formulated and the parameterization defined (here, $S(x)$ is described by Bezier–Bernstein polynomials), the corresponding software was programmed and used for validation purposes. A characteristic example is shown in fig. 1, where the same quasi $1D$ duct was redesigned using known (a) pressure, (b) velocity and (c) density distributions along x, as targets. The minimization method was a steepest descent algorithm using the gradient computed by the adjoint method.

3 Adjoint Formulation for $3D$ flows

Though the proposal was exclusively dealing with $2D$ applications, it was decided to proceed to the formulation of the $3D$ adjoint equations. The $2D$ case should be considered as a simple counterpart of the $3D$ one. The basic differences of the $2D$–$3D$ formulations in contrast to the quasi $1D$ one is the fact that the target is defined at the boundary of the computational domain which results in the inadmissibility of certain objective functionals, and in particular, those which are not expressions as function of pressure.

The objective function in the case of the inverse design of a $3D$ aerodynamic shape is written as

$$F = \int\int_{surface} (p(s) - p_{tar}(s))^2 ds \tag{9}$$

The Euler Equations for $3D$ flows read

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{f}}{\partial x} + \frac{\partial \vec{g}}{\partial y} + \frac{\partial \vec{j}}{\partial z} + \vec{q} = \vec{0} \tag{10}$$

where $\vec{U} = [\rho \; \rho u \; \rho v \; \rho w \; E]^T$, $\vec{f} = \left[\rho u \quad \rho u^2 + p \quad \rho uv \quad \rho uw \quad u\,(E+p)\right]^T$, $\vec{g} = \left[\rho v \quad \rho uv \quad \rho v^2 + p \quad \rho vw \quad v\,(E+p)\right]^T$, $\vec{j} = \left[\rho w \quad \rho uw \quad \rho vw \quad \rho w^2 + p \quad w\,(E+p)\right]^T$ and $\vec{q} = \left[0 \quad -\rho(2\omega v + \omega^2 x) \quad +\rho(2\omega u - \omega^2 y) \quad 0 \quad 0\right]^T$, where ω is the rotational velocity.

Since this research was carried out in a turbomachinery lab., it was considered useful to maintain rotational terms; so, the proposed method operates for either stationary or rotating frames of reference. The augmented objective functional is written as

$$F_{aug} = F - F_c = F - \int\int\int_{\mho} \vec{\Psi}^T \left(\frac{\partial \vec{f}}{\partial x} + \frac{\partial \vec{g}}{\partial y} + \frac{\partial \vec{j}}{\partial z} + \vec{q} \right) d\mho \tag{11}$$

and its variation results in the field adjoint equations

$$\frac{\partial \vec{\Psi}}{\partial t} - A^T \frac{\partial \vec{\Psi}}{\partial x} - B^T \frac{\partial \vec{\Psi}}{\partial y} - C^T \frac{\partial \vec{\Psi}}{\partial z} + \vec{q}_{\Psi} = \vec{0} \tag{12}$$

where $\vec{q}_{\Psi} = \left[0 \quad -(2\omega\Psi_3 + \omega^2 x \Psi_1) \quad +(2\omega\Psi_2 - \omega^2 y \Psi_1) \quad 0 \quad 0\right]$ and A, B, C are the Jacobian matrices of flow fluxes. The adjoint boundary conditions are

$$A_n{}^T \vec{\Psi} = \vec{0} \tag{13}$$

where $A_n = An_x + Bn_y + Cn_z$. The wall surface boundary condition is proved to be

$$(p - p_{tar}) + \Psi_2 n_x + \Psi_3 n_y + \Psi_4 n_z = 0 \tag{14}$$

in the case of the pressure–target. The compatibility relations for the inadmissible cost functions, dealing with a velocity or density target distribution are found to be

$$(V - V_{tar}) - \rho V (\Psi_2 n_x + \Psi_3 n_y + \Psi_4 n_z) = 0 \tag{15}$$

$$(\rho - \rho_{tar}) + c^2 (\Psi_2 n_x + \Psi_3 n_y + \Psi_4 n_z) = 0 \tag{16}$$

The sensitivity derivative expression is

$$
\begin{aligned}
\delta F_{aug} \;=\;& \frac{1}{2}\iint_{(w)} (p - p_{tar})^2 \delta(ds) \\
-& \iint_{(w)} \left(\rho u \Psi_1 + \rho u^2 \Psi_2 + \rho u v \Psi_3 + \rho u w \Psi_4 + u(E_t + p)\Psi_5\right) \delta(n_x ds) \\
-& \iint_{(w)} \left(\rho v \Psi_1 + \rho u v \Psi_2 + \rho v^2 \Psi_3 + \rho v w \Psi_4 + v(E_t + p)\Psi_5\right) \delta(n_y ds) \\
-& \iint_{(w)} \left(\rho w \Psi_1 + \rho u w \Psi_2 + \rho v w \Psi_3 + \rho w^2 \Psi_4 + w(E_t + p)\Psi_5\right) \delta(n_z ds) \\
+& \iiint_{\mho} \vec{\Psi}^T \left(\frac{\partial \vec{f}}{\partial \xi}\delta(\xi_x) + \frac{\partial \vec{f}}{\partial \eta}\delta(\eta_x) + \frac{\partial \vec{f}}{\partial \zeta}\delta(\zeta_x)\right) d\mho \\
+& \iiint_{\mho} \vec{\Psi}^T \left(\frac{\partial \vec{g}}{\partial \xi}\delta(\xi_y) + \frac{\partial \vec{g}}{\partial \eta}\delta(\eta_y) + \frac{\partial \vec{g}}{\partial \zeta}\delta(\zeta_y)\right) d\mho \\
+& \iiint_{\mho} \vec{\Psi}^T \left(\frac{\partial \vec{j}}{\partial \xi}\delta(\xi_z) + \frac{\partial \vec{j}}{\partial \eta}\delta(\eta_z) + \frac{\partial \vec{j}}{\partial \zeta}\delta(\zeta_z)\right) d\mho
\end{aligned}
\tag{17}
$$

4 Method Application–Indicative Results

At the final stage of this research project, the $2D$ and $3D$ adjoint equations and boundary conditions, as previously exposed in brief, were programmed. It is obvious that an adjoint inverse design method needs to be based on a flow solution software. As such, we used an existing finite–volume, time–marching, Euler equations solver which can also take into account rotating frame of references. The adjoint equations solver was programmed in a form compatible with the aforementioned flow solver and was linked to NURBS parametric representations for the $3D$ shapes (i.e. blades, in the few results shown in this summary report).

Since the major scope of the undertaken research was the adjoint formulation (rather than its use for optimization) it is important to demonstrate the accuracy with which the adjoint method computed the gradient of the objective function. So, fig. 2 compares the objective function gradient as predicted (a) by central–finite differences and (b) by the adjoint method. These figures correspond to $2D$ shape designs; in both of them, the target is a known pressure distribution along the shape contour. The horizontal axis corresponds to the design variables, one by one. In both cases, the accuracy with which the adjoint method predicts the gradient is very satisfactory. Note that the gradient component values predicted by the finite–differences are considered as reference values, since a parametric investigation was carried out in advance (not shown here).

Since one of the aims of an "oriented basic research" program is to foresee and try to solve future

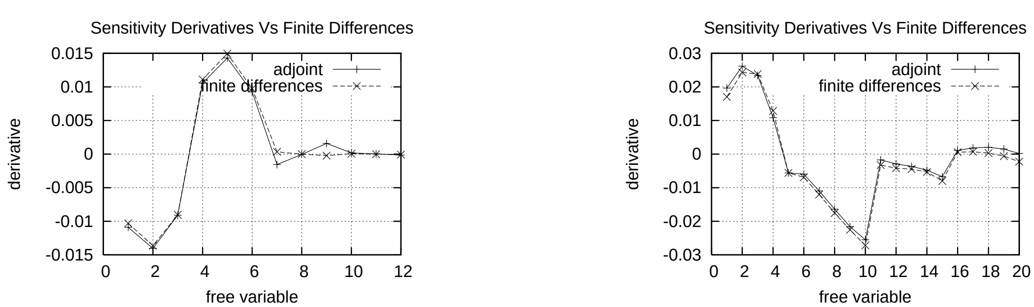

Figure 2: Comparison of the adjoint sensitivity derivatives with the central finite differences in the case of a $2D$ airfoil (left) and a $2D$ compressor blade (right).

problems, a number of real world design problems (with hypothetical data) have been worked out and these are shown in figs. 3. The caption of each figure explains briefly each problem considered.

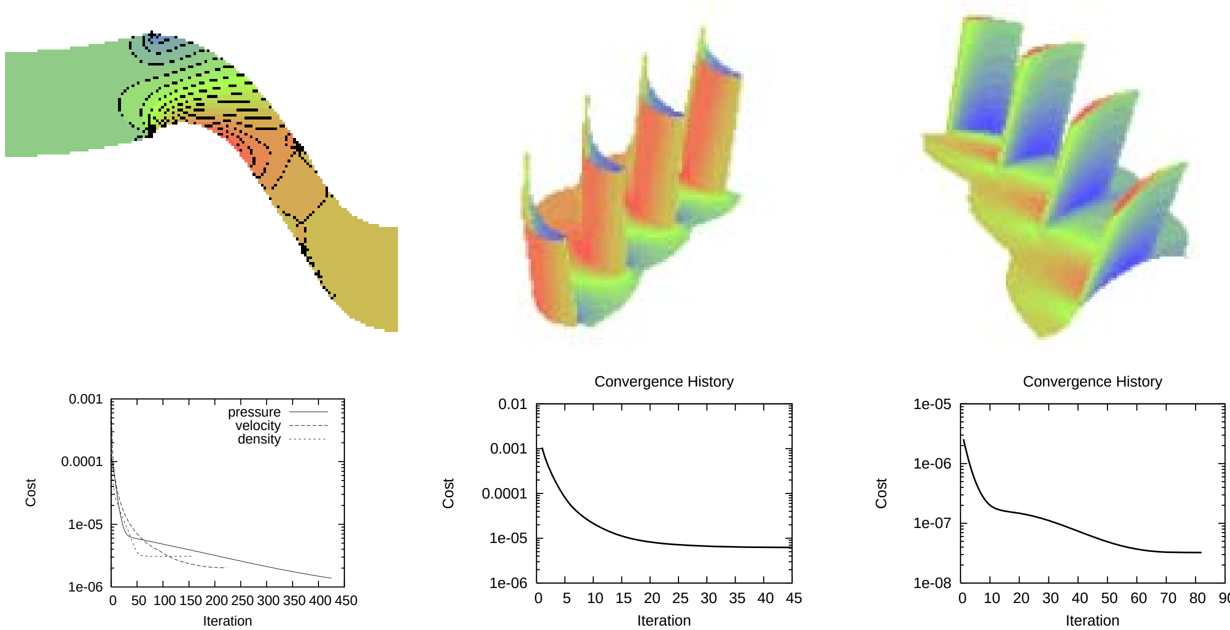

Figure 3: Left: $2D$ turbine cascade inverse design; $M_{2_{is}} = 0.5$, middle: $3D$ peripheral turbine cascade inverse design; $M_{2_{is}} = 0.45$, $\alpha_{per,1} = 19.3^o$, $\alpha_{rad,1} = 0^o$, right: $3D$ rotational compressor cascade inverse design; $M_{2_{is}} = 0.45$, $\alpha_{per,1} = 0^o$, $\alpha_{rad,1} = 0^o$. Top: Mach number isolines for the target geometry, bottom: convergence of the steepest descent algorithm (The inadmissible cases convergence rates are included in the first figure).

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