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A Discrete Adjoint Formulation for Inviscid Flow Nozzle Optimization

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Abstract

A discrete adjoint formulation with an ad hoc flow solver has been recently developed and tested on transonic inviscid flow optimization problems. In the present paper the formulation is extended to compressible as well as incompressible flow solvers. First, the adjoint equations are coupled with an accurate in-house flow solver to test the approach on some inverse design problems involving two- and three-dimensional transonic and subsonic flows. Then, the previous design test cases are re-computed coupling the extended adjoint formulation with commercial and open source flow solvers, without noticing any relevant difference in the optimization convergence histories. Finally, incompressible design test cases are successfully computed by means of commercial solver for incompressible flows. The extended compressible adjoint formulation appears to have a wide application, insofar as it allows to perform accurate and efficient design optimization using different flow conditions, different flow solvers and even a solver for incompressible flows.

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Keywords: Shape optimization; Adjoint equations; Nozzle; Inviscid flow.

1. Introduction

As discussed in Ref. [1], fluid dynamic design procedures generally require the calculation of many computationally expensive flow analyzes. Most approaches are based upon a sequence of global iterations, each one of them requiring a computation of the converged flow field, a solution for the sensitivity derivatives and an appropriate update of the design parameters. The high computational cost of this serial approach comes principally from the repeated solution of flow equations. In contrast, Ref.[1] has introduced a progressive optimization strategy, whereby the optimization process is based on partially converged flow solutions with the aim to converge the flow solution while converging the design problems. This strategy has been applied to the computation of some two-dimensional flow op-

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timization problems and has been compared to serial convergence strategy, showing a reduction of the computational effort by a factor of 50.

Ref. [2], examines issues related to developing robust sensitivity derivatives using an adjoint formulation based on an approximate flow solver, particularly effective for situations when the objective function is noisy or non-smooth. The efficiency of this smoothing procedure and of the progressive optimization strategy has been shown in Ref. [3], which considered the extension of the methodology to three-dimensional inviscid flow problems. The extension to viscous airfoil design problems has been presented in Ref. [4], where adjoint equations based on an inviscid flow formulation have been employed to compute inverse and direct test cases on laminar as well as turbulent transonic airfoils.

The smoothing procedure (Ref. [2]) and the use of partially converged solutions of flow and adjoint equations imply that the optimization process is based on approximate values of the gradient of the objective function. Another example of approximate design sensitivity has been discussed by Matsuzawa and Hafez (Ref. [5]), where adjoint equations based on an inviscid flow formulation have been used to determine approximate gradients of the objective function for airfoil inverse design in laminar flow conditions.

The progressive optimization strategy of Ref. [3] used only an ad hoc flow solver, which was coupled with the suggested adjoint equations to compute transonic flow design problems. The aim of the present paper is to develop a general use discrete adjoint method to be combined with different flow solvers for the inverse design optimization of two- and three-dimensional inviscid flow problems. Some preliminary results have been presented in Ref. [6]; here the optimization tests are extended to different flow solvers to enhance the wide applicability of the methodology.

First, we will present the formulation of Ref. [3], together with the suggested modifications, introducing the objective function, the adjoint formulation and the progressive optimization strategy. The adjoint formulation will be coupled with a flow solver developed in-house, a commercial flow solver and an open source flow solver. The suggested method will be applied to the inverse design of two- and three-dimensional nozzles (Ref. [7, 8, 9]) in transonic and subsonic flow conditions. Finally, the compressible adjoint formulation will be coupled with a solver for incompressible flow and applied to the design of the same two- and three-dimensional nozzles in incompressible flow conditions.

2. Formulation

The inverse design of nozzles consists of finding the geometric shape whose computed pressure distribution along the wall, $p_i(\boldsymbol{\xi})$, matches a target pressure distribution, $\hat{p}_i$ in discrete form. The corresponding discrete objective function, $I(\boldsymbol{\xi})$, may be defined as:

$$I(\boldsymbol{\xi}) = \frac{1}{2\,N_c} \sum_{i=1}^{N_c} [p_i(\boldsymbol{\xi}) - \hat{p}_i]^2, \tag{1}$$

where $\boldsymbol{\xi}$ represents the design parameters, while N_c indicates the number of linear (in 2D cases) or surface (in 3D cases) intervals used to discretize the wall surface.

All the flow computations are performed using three different basic flow solvers. The first one has been developed in-house; it is based on the finite-volume, flux-difference-splitting method of Roe (Ref. [10]), in order to accurately capture shock waves. The second flow solver is provided by the commercial software ANSYS FLUENT (version 14.5); it is based on a flux-vector splitting scheme, called Advection Upstream Splitting Method (AUSM), which was first introduced by Liou and Steffen in Ref. [11]. The third flow solver is provided by the release 2.2.2 of the open source software OpenFOAM (Open Field Operation and Manipulation), an open source library designed for development of multi-dimensional modeling codes. In particular, we use the pressure-velocity coupled solver for compressible transient transonic/subsonic flows, called SonicFoam (Ref. [12]). For the incompressible flow tests we use the SIMPLE solver for incompressible flows, provided by ANSYS FLUENT. SIMPLE (Ref. [13]) is the acronym of Semi-Implicit Method for Pressure-Linked Equations.

The computational flow field is divided into an $N \times M$ finite-volume mesh for two-dimensional flow applications while an $N \times M \times K$ finite-volume mesh is employed for three-dimensional flows, where N is the number of intervals in the streamwise direction, M the number of intervals in the first crossflow direction, K the number of intervals in the second crossflow direction (only for 3D flows).

The discrete adjoint formulation of Ref. [3] is based on an auxiliary flow solver used only for the computation of smooth sensitivity derivatives. The employed solver is based on a central scheme with an adequate level of numerical viscosity. For example, within the context of a three-dimensional Cartesian finite-volume formulation, we can modify the flux at a generic $(m+1/2,\ n,\ l)$ cell edge with the introduction of a numerical viscosity flux $\mathbf{D}_{m+1/2,n,l}$, given by:

$$\mathbf{D}_{m+1/2,n,l} \ = \ d_{m+1/2,n,l}\,(\mathbf{q}_{m+1,n,l} \ - \ \mathbf{q}_{m,n,l}), \tag{2}$$

where d is the coefficient of artificial viscosity. The vector of conserved variables, $\mathbf{q}$, for a three dimensional problem is given by:

$$\mathbf{q} \ = \ [\rho,\ \rho u,\ \rho v,\ \rho w,\ \rho e_o]^T, \tag{3}$$

where p, ρ, u, v, w, e_o are the pressure, the density, the three Cartesian components of the velocity vector, and the total internal energy, respectively.

According to Ref. [3], the sensitivity derivatives of the objective function, $I(\boldsymbol{\xi})$, with respect to the design parameters $\boldsymbol{\xi}$ can be expressed as:

$$\frac{\partial I}{\partial \xi_j} = \left(\frac{\partial I}{\partial \xi_j}\right)_{\mathbf{u}} - \mathbf{\Lambda}_k^T \left(\frac{\partial \mathbf{w}_k}{\partial \xi_j}\right)_{\mathbf{u}}, \tag{4}$$

where:

$$\mathbf{w}_k(\mathbf{u},\boldsymbol{\xi}) \ = \ 0. \tag{5}$$

represents the discretized system of governing partial differential equations corresponding to the auxiliary flow solver. Note that the adjoint variables $\mathbf{\Lambda}$ represent a vector of four (five for 3D cases) auxiliary variables defined at each cell center of the computational mesh, evaluated by solving the adjoint equations:

$$\left(\frac{\partial \mathbf{w}_k}{\partial \mathbf{u}_i}\right)_{\xi}^T \mathbf{\Lambda}_k \ = \ \left(\frac{\partial I}{\partial \mathbf{u}_i}\right)_{\xi}^T, \tag{6}$$

for $i = 1,\ldots,N\times M$ ($i = 1,\ldots,N\times M\times K$ for 3D test cases), $j = 1,\ldots,n$, with n the number of design parameters and repeated indices k summed over their range. Moreover, the vector of physical variables $\mathbf{u}_i$ at each cell center, i, for a three dimensional problem is given by:

$$\mathbf{u}_i \ = \ [p,\ \rho,\ u,\ v,\ w]_i^T. \tag{7}$$

Note that the terms $(\partial I/\partial \mathbf{u}_i)_{\xi}$ and $\left(\partial I/\partial \xi_j\right)_{\mathbf{u}}$ can generally be evaluated directly from the definition of the objective function itself. Likewise, the terms $(\partial \mathbf{w}_k/\partial \mathbf{u}_i)_{\xi}$ and $\left(\partial \mathbf{w}_k/\partial \xi_j\right)_{\mathbf{u}}$ can generally be evaluated directly from the definition of the system of algebraic equations, Eqs. (5), and depend on the solution of the flow field.

Eqs. (6) represent the adjoint equations, which can generally be used to evaluate the adjoint variables with a direct solver, for two-dimensional application. For three-dimensional flow problems, this direct solver may be comparatively too expensive in terms of CPU time consuming. In such cases, an alternative solution may be devised: Eqs. (6) are modified by introducing additional terms representing the time derivative, $\partial \mathbf{\Lambda}_i/\partial t$, of the adjoint variables, in order to devise a pseudo-time dependent iterative solver:

$$\frac{\partial \mathbf{\Lambda}_i}{\partial t} + \left(\frac{\partial \mathbf{w}_k}{\partial \mathbf{u}_i}\right)_{\xi}^T \mathbf{\Lambda}_k \ = \ \left(\frac{\partial I}{\partial \mathbf{u}_i}\right)_{\xi}^T. \tag{8}$$

In the practical applications the procedure is the following. The physical variables are first computed with one of the basic flow solvers. Then they are used to compute the terms $(\partial I/\partial \mathbf{u}_i)_{\xi}$ and $(\partial \mathbf{w}_k/\partial \mathbf{u}_i)_{\xi}$. Finally, Eqs. (6) or Eqs. (8) are solved for the adjoint variables, $\mathbf{\Lambda}$, and Eqs. (4) are used to evaluate the sensitivity derivatives.

The goal of the progressive optimization technique is to simultaneously determine the minimum of the objective function, while progressively reaching a converged solution for the flow field. The optimization procedure starts the computation on a coarse grid, partially converging the flow solution and computing the sensitivity derivatives. Then, the design parameters at the $l + 1$ optimization step are updated according to the relation:

$$\xi_j^{l+1} = \xi_j^l - a_j \frac{\partial I}{\partial \xi_j}, \tag{9}$$

where a_j are positive variables. The previous steps are repeated until the gradient of the objective function is decreased one to two orders of magnitude, while gradually converging the flow solution. Next, the mesh is refined and the previous optimization steps are repeated until the finest grid is reached and the gradient of the objective function has sufficiently decreased. In the computed results, we have observed the objective function to be sufficiently decreased when the norm of its gradient has decreased 2.5 orders of magnitude with respect to its value after the first optimization step.

The variations of the sensitivity derivatives in two subsequent optimization steps have been limited when applying commercial flow solvers. Indeed, they may cause relevant wiggles, which significantly change according to small geometry variations. This event may cause large sensitivity derivative jumps in two subsequent global steps, thus impairing the smoothness required by a progressive optimization strategy. Consequently, we have limited the modulus of each sensitivity derivative to be no more than the double of the value assumed in the previous optimization global step.

3. Two-Dimensional Nozzle Results

The first test case considered is the flow in a straight 2D nozzle with a symmetry line located at $y = 1$. The lower wall ordinates, y_w, are zero for $-0.5 \leq x \leq 0$ and $1 \leq x \leq 1.5$, while in the range $0 \leq x \leq 1$ they are defined as follows:

$$y_w(x) = \sum_{i=1}^{N_a} \alpha_i \, x^{i+1} \, (x - 1)^2, \tag{10}$$

where N_a is the number of the design parameters α_i. According to Refs. [7] and [8], we have assumed $\alpha = (2, 0, 0, 0)$ to define the target lower wall geometry, which has been used to determine the target pressure distribution along the lower wall. The computations have been performed by progressively employing three mesh levels made by 20×5, 40×10, 80×20 cells. The flow field is evaluated by employing an H grid defined by $(x_l, y_m) = (x_o + l\Delta x, y_w + m\Delta y)$, where Δx is constant and Δy is a constant fraction of the local height of the channel.

We have coupled the proposed adjoint formulation with compressible flow solvers to perform optimization tests with transonic and subsonic flow conditions employing 1, 4 and 20 design parameters. Finally, the proposed compressible adjoint formulation, developed for design optimization in compressible flow conditions, has been coupled with an incompressible flow solver to check if the adjoint formulation can be extended to effective incompressible flows. For the transonic test case, the outlet pressure, adimensionalized with respect to the inlet total pressure, is equal to 0.7, while it is equal to 0.9 for the subsonic case and to 0.992 for the incompressible flow solver case.

The isoMach lines corresponding to the target lower wall geometry are shown in Fig. 1, where a small supersonic flow bubble located in the bump region and terminated by a recompression shock can be observed. Figs. 2, 3 and 4 show the target pressure distribution (continuous line), the initial pressure distribution (dashed line) and the converged pressure distribution (symbols) for the transonic, the subsonic and the incompressible test cases, respectively. We have computed the work units required by the three flow types, by the employed flow solvers and by the different design parameter (DP) to converge the gradient of the objective function by 2.5 order of magnitude. The results are reported in Table 1. A unit of work is the computational time required to run a single flow analysis on the finest mesh of the considered flow solver with a drop in the residuals equal to 5 orders of magnitude.

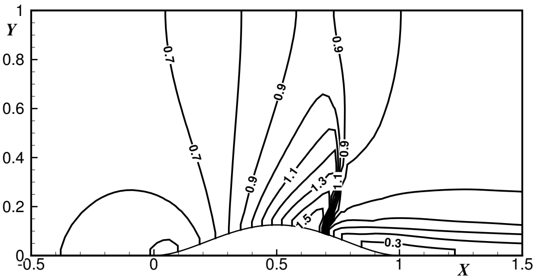

Fig. 1. Target isoMach lines. Transonic 2D nozzle.

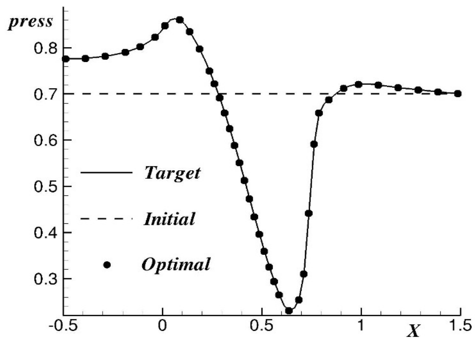

Fig. 2. Pressure distribution. Transonic 2D nozzle. OpenFOAM flow solver. 4 design parameters.

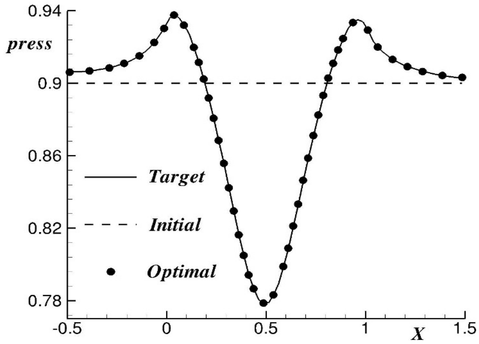

Fig. 3. Pressure distribution. Subsonic 2D nozzle. FLUENT AUSM flow solver. 4 design parameters.

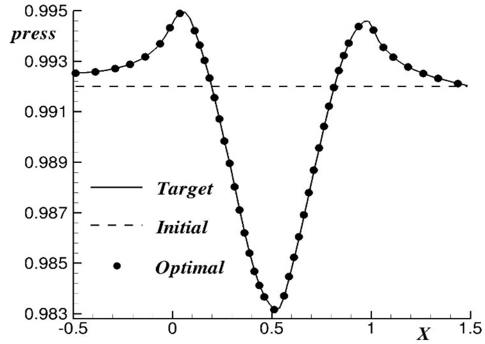

Fig. 4. Pressure distribution. FLUENT SIMPLE incompressible flow solver. 20 design parameters.

Table 1. Work units required for the 2D nozzle flows.

Flow Type	Flow Solver	1 DP	4 DP	20 DP
Transonic Flow	In-house flow solver	0.69	1.21	1.26
	FLUENT AUSM flow solver	0.22	0.51	0.95
	OpenFOAM SonicFoam flow solver	1.08	1.71	2.32
Subsonic Flow	In-house flow solver	0.45	3.00	4.50
	FLUENT AUSM flow solver	0.34	3.30	3.98
	OpenFOAM SonicFoam flow solver	2.53	3.65	4.44
Incompressible Flow	FLUENT SIMPLE flow solver	1.32	4.49	7.83

4. Three-Dimensional Nozzle Results

The three-dimensional test case considered is the flow in a straight three-dimensional nozzle with a symmetry plane, located at $y = 1$. The geometry and the finest employed mesh are shown in Fig. 5. Calculations have been performed only on the lower half of the nozzle. The shape of the lower wall, corresponding to the nozzle profile, is quite similar to the one used in Ref. [9] for this type of geometries. The wall ordinates are zero for $-0.5 \leq x \leq x_{in}$ and $(1 + x_{in}) \leq x \leq 2.5$, while in the range $x_{in} \leq x \leq (1 + x_{in})$ they are defined as follows:

$$y_w(x,z) = \sum_{i=1}^{N_a} \alpha_i \, (x - x_{in})^{i+1} \, [x - (1 + x_{in})]^2, \tag{11}$$

where:

$$x_{in} = \sum_{i=1}^{N_b} \beta_i \, (z - z_{max}/2)^i. \tag{12}$$

Note that N_a and N_b are the number of the design parameters α_i and β_i, respectively. The front and rear walls are located at $z_{min} = 0$ and $z_{max} = 1$. The target geometry corresponds to $\alpha_1 = 2$ and $\beta_1 = 0.51$, while the other α_i and β_i values are set to 0. The computations have been performed by progressively employing three mesh levels made by $16 \times 4 \times 4$, $32 \times 8 \times 8$, $64 \times 16 \times 16$ cells. The flow field is evaluated by employing an H grid defined by $(x_l, \ y_m, \ z_n) = (x_o + l\Delta x, \ y_w + m\Delta y, \ z_o + n\Delta z)$, where Δx and Δz are constant and Δy is a constant fraction of the local height of the channel. The computed pressure distribution on the lower wall is assumed as the target pressure.

We have considered optimization tests with transonic and subsonic flow conditions employing 5, 8, 20 and 40 design parameters. Finally, the proposed compressible adjoint formulation has been coupled with an incompressible flow solver. For the transonic test case , the outlet pressure, adimensionalized with respect to the inlet total pressure, is equal to 0.7, while it is equal to 0.9 for the subsonic case and to 0.992 for the incompressible flow solver case.

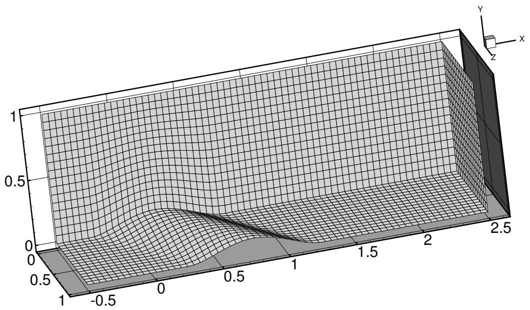

Fig. 5. Three-dimensional nozzle geometry.

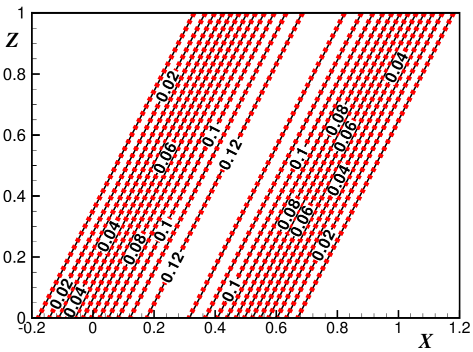

Fig. 6. Target and optimized lower wall isolevel lines. Transonic 3D nozzle. OPENFOAM flow solver. 40 design parameters.

Fig. 6 shows that the optimal lower wall isolevel lines (red dashed lines) practically coincide with the target ones (dark continuous lines). Figs. 7 and 8 show the optimal isobars on the nozzle lower wall (red dashed lines) and the target ones (dark continuous lines) for the subsonic and the incompressible test cases, respectively. The work units required to converge the gradient of the objective function by 2.5 order of magnitude are reported in Table 2, for the three flow types.

5. Result discussion

The results of all the compressible test cases (see Tables) allow to state that the optimization process can be performed using the proposed adjoint formulation coupled with three different compressible flow solvers, operating in transonic and subsonic flow conditions. The work units required by the different flow solvers to converge the objective function by 2.5 orders of magnitude do not show major differences in most cases. The work required is slightly higher than one unit in most cases and even lower than one unit in some cases, because of the efficiency of the mesh sequencing. We also observe a small increase of the required work when increasing the number of design variables in most cases while a small decrease can be observed in a few cases thus proving that increasing the number of the design variables does not significantly impair the convergence properties of the present technique.

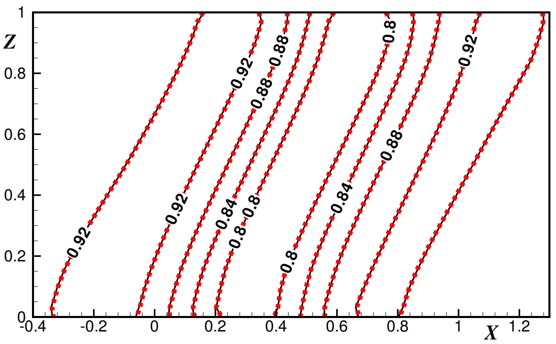

Fig. 7. Target and optimized isobars on the lower wall. Subsonic 3D nozzle. FLUENT AUSM flow solver. 20 design parameters.

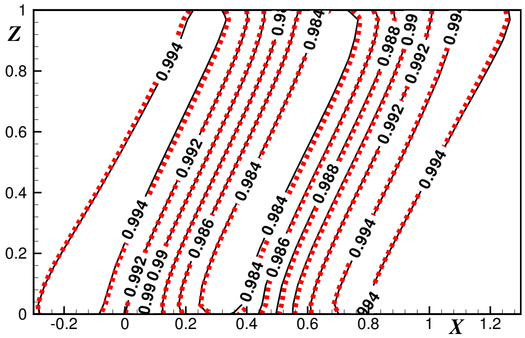

Fig. 8. Target and optimized isobars on the lower wall. Incompressible 3D nozzle. FLUENT SIMPLE incompressible flow solver. 40 design parameters.

Table 2. Work units required for the 3D nozzle flows.

Flow Type	Flow solver	5 DP	8 DP	20 DP	40 DP
Transonic Flow	In-house flow solver	0.43	0.48	0.77	0.75
	FLUENT AUSM flow solver	0.99	0.89	1.25	1.40
	OpenFOAM SonicFoam flow solver	1.15	1.05	2.10	2.38
Subsonic Flow	In-house flow solver	0.80	1.01	1.14	0.91
	FLUENT AUSM flow solver	1.96	0.72	2.51	1.99
	OpenFOAM SonicFoam flow solver	0.90	1.20	1.70	1.26
Incompressible Flow	FLUENT SIMPLE flow solver	19.6	19.7	21.4	22.5

Figs. 2 and 3 show the optimal and the target pressure distributions for two different 2D test cases. These figures prove that the optimized pressure distribution practically coincides with the target one. For the transonic test case (Fig. 2), the coincidence in the very sensitive shock transition region is particularly relevant. This coincidence indicates that the solution has sufficiently converged for all the considered test cases. Fig. 7 shows a similar coincidence of the optimal isobars with the target isobars for the 3D subsonic test case, thus outlining the effective optimization convergence for the present 3D test case too. The same conclusion on the optimization convergence can be deduced from Fig. 6, which shows the practical coincidence of the optimal isolevel lines with the target ones for the 3D transonic test case.

Finally, we refer to Figs. 4 and 8 and to the last line of Tables 1 and 2, which refer to the optimization of incompressible flow test cases by means of an incompressible flow solver. These figures and tables reinforce the conclusions pertaining to compressible flow test cases. In particular they allow to state that design optimizations can be performed using the proposed compressible adjoint formulation coupled with a solver for incompressible flows.

The computed results allow to stress the conclusion that the proposed adjoint formulation can be coupled with compressible solvers independently of the numerical approach used to solve the flow. More importantly we can emphasize that the proposed adjoint formulation developed for compressible flow design tests can even be coupled with a solver for incompressible flows to solve incompressible flow design problems.

6. Conclusions

A general purpose discrete adjoint formulation for robust and efficient design optimization in compressible and incompressible inviscid flow conditions, with different flow solvers, is presented and tested on two- and three-dimensional compressible and incompressible nozzle flow problems.

The methodology has five essential ingredients. First, approximate but efficient design sensitivities are obtained using a discrete adjoint formulation. The adjoint problem is based on a dissipative compressible flow solver in order to obtain robust sensitivity derivatives in presence of noise or other non-smoothness associated with objective functions in many high-speed flow problems. The second ingredient involves what we term *progressive optimization*, whereby a sequence of a partially converged flow solution, followed by an optimization step is performed. The third ingredient is the use of progressively finer grids for the progressive solution of the flow field. The fourth ingredient is the use of accurate flow solvers. The fifth ingredient is the limit imposed to the sensitivity derivative variations to preserve the smoothness of the progressive procedure in presence of wiggles typical of transonic flows computed using commercial solvers.

This approach has been tested on transonic and subsonic inviscid flow optimization tests, referring to two- and three-dimensional nozzles, computed with different numbers of design parameters. We have performed the previous computations employing an accurate in-house flow solver, a commercial flow solver, provided by the commercial software ANSYS FLUENT and an open source flow solver provided by the software OpenFOAM. No significant difference with respect to the results computed by means of the in-house flow solver has been observed for some of the test cases, while some other test runs have shown a faster or slower convergence. These results prove the employed adjoint formulation to be quite general, because it allows to perform design optimizations using different flow solvers. Moreover, the efficiency of the procedure is not significantly impaired when the number of design parameters is increased.

Finally, we have successfully computed incompressible two- and three-dimensional nozzle test cases coupling the extended compressible adjoint formulation with a solver for incompressible flows. The suggested discrete adjoint formulation has been developed for design optimization in compressible flow conditions. Nevertheless, it has been coupled with a solver for incompressible flows and has allowed to successfully compute optimization test cases. This finding further substantiates the conclusion the suggested compressible discrete adjoint formulation to be a general purpose adjoint formulation, which can even be coupled with incompressible flow solvers.

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