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ON THE BOUNDARY COMPUTATION OF FLOW SENSITIVITIES

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Abstract

A methodology to deal with shape optimization in flow problems is described. The scheme is based on the solution of a continuous adjoint problem. The computation of the objective function sensitivities is performed by using only the flow and adjoint solutions **on the boundary**. This property makes the scheme totally independent of the numerical solvers (flow and adjoint). In addition, the scheme allows the use of incomplete gradients by only taking into account the geometrical sensitivities, and/or the boundary conditions of the adjoint problem. The error generated by this procedure is well stablished in the paper. Finally, an improved pseudo-shell approach to move the surface to be optimized, and to impose the geometric restrictions is proposed and tested. Some applications for control and design problems are shown.

1 Introduction

The general optimization problem can be formulated as follows:

$$\text{Min } I(\boldsymbol{U},\boldsymbol{\beta}) \quad \text{subject to} \quad \boldsymbol{G}(\boldsymbol{U},\boldsymbol{\beta}) \leq \boldsymbol{0} \quad \text{and} \quad \boldsymbol{R}(\boldsymbol{U},\boldsymbol{\beta}) = \boldsymbol{0} \quad \text{in} \quad \Omega \ , \tag{1}$$

where I is the objective function to be minimized (i.e. drag, target pressure, etc,), $\boldsymbol{U}$ and $\boldsymbol{\beta}$ are the flow variables (velocities, pressures, etc,) and the design parameters, respectively. $\boldsymbol{G}$ stands for the geometric and flow constraints (constant enclosed volume, design parameter ranges, constant lift, etc,), and $\boldsymbol{R}$ are the continuous flow equations. Ω is the flow domain, which will vary in the optimization process, and is parameterized through the design variables $\boldsymbol{\beta}$. A variation of the objective function due to a variation of Ω (named $\delta\Omega$) will be given by:

$$\delta I = \frac{\partial I}{\partial \boldsymbol{\beta}}\delta\boldsymbol{\beta} + \frac{\partial I}{\partial \boldsymbol{U}}\delta\boldsymbol{U} \ . \tag{2}$$

In most cases the first right hand side term of (2) can be computed analytically or via finite differences in a straightforward manner. On the other hand, the computation of the second one is more involved, as it is related to $\boldsymbol{\beta}$ through the flow equations.

A method to overcome this shortcoming is via the **adjoint problem** [16, 17, 4, 20, 7, 19, 15, 2, 3, 9, 1, 18, 21, 5, 13, 14, 12, 23, 24, 25, 8, 27]. With this scheme some adjoint variables (or Lagrange multipliers) $\boldsymbol{\Psi}$ are introduced over the flow domain, and the objective function is reformulated as:

$$L(\boldsymbol{U},\boldsymbol{\beta}) = I(\boldsymbol{U},\boldsymbol{\beta}) + \int_\Omega \Psi \cdot \boldsymbol{R} \ . \tag{3}$$

Then, the variation of L due to a change in domain $\delta\Omega$ is given by:

$$\begin{aligned} \delta L &= \Big(\frac{\partial I}{\partial \boldsymbol{\beta}} + \int_\Omega \boldsymbol{\Psi}\cdot\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\beta}}\Big)\delta\boldsymbol{\beta} \\ &+ \Big(\frac{\partial I}{\partial \boldsymbol{U}} + \int_\Omega \boldsymbol{\Psi}\cdot\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}}\Big)\delta\boldsymbol{U} \ . \end{aligned} \tag{4}$$

By choosing $\boldsymbol{\Psi}$ in such a way that:

$$\frac{\partial I}{\partial \boldsymbol{U}}\delta\boldsymbol{U} + \int_\Omega \boldsymbol{\Psi}\cdot\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}}\delta\boldsymbol{U} = 0 \ , \tag{5}$$

δL can be computed by the remaining terms of (4). Note that such a procedure is independent of the number of design parameters, and only depends on the number of

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objective functions to be minimized (or maximized). For this reason, it is probably the best option for flow optimization problems, where objective functions are expensive to evaluate and many design parameters are present.

2 Gradient Computations

As stated before, the partial derivative of the original objective function with respect to the design parameters (first term of (4)) is computed in a straighforward manner (analytically or via finite differences). This leaves the remaining term in equation (4), namely

$$\int_\Omega \boldsymbol{\Psi} \cdot (\partial \boldsymbol{R}/\partial \boldsymbol{\beta}) \delta \boldsymbol{\beta}. \tag{6}$$

The first option is to evaluate it via finite differences (the flow remains constant in such a calculation). This has been our common practice until this moment [23, 24, 25, 8]. However, this procedure is intimately linked to the numerical scheme used to obtain the flow solution, and is also computationally intensive, involving the equivalent of approximately 300 explicit timesteps with geometry recalculations. If one could recast the volume integral as a boundary integral, the adjoint and flow solvers could be treated independently, and the computational expense would be reduced significantly. With this objective in mind, it can be noticed that the gradient term of (6) can be expanded as:

$$\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\beta}_m} \delta \boldsymbol{\beta}_m = \boldsymbol{R}(\boldsymbol{U}(\boldsymbol{\beta}_m + \delta \boldsymbol{\beta}_m)) - \boldsymbol{R}(\boldsymbol{U}(\boldsymbol{\beta}_m)) \quad , \tag{7}$$

and that $\boldsymbol{U}(\boldsymbol{\beta}_m + \delta\boldsymbol{\beta}_m)$ ($m = 1, ..., n_{\mathrm{dp}}$ with n_{dp} the number of design parameters) can be computed by the following Taylor series expansion:

$$\boldsymbol{U}(\boldsymbol{\beta}_m + \delta \boldsymbol{\beta}_m) = \boldsymbol{U}(\boldsymbol{\beta}_m) + \delta \boldsymbol{\beta}_m \cdot \nabla \boldsymbol{U} + O(\delta\beta^2) \quad . \tag{8}$$

Hence, if the design parameters are allowed to move only in the normal direction of the objective function support (surface to be optimized $\mathcal{S}$), $\delta\boldsymbol{\beta}_m$ can be expressed as:

$$\delta \boldsymbol{\beta}_m = -\epsilon \boldsymbol{n} \quad , \tag{9}$$

where $\boldsymbol{n}$ is the exterior normal to $\mathcal{S}$ at $\boldsymbol{x}_m$ (spatial position of $\boldsymbol{\beta}_m$), and $0 < \epsilon << 1$ is a real constant. Now, equation (8) is re-written as:

$$\begin{aligned} \boldsymbol{U}(\boldsymbol{\beta}_m - \epsilon \boldsymbol{n}) &= \boldsymbol{U}(\boldsymbol{\beta}_m) - \epsilon \boldsymbol{n} \cdot \nabla \boldsymbol{U} + O(\epsilon^2) \\ &\approx \boldsymbol{U} + \delta \boldsymbol{U} \quad . \end{aligned} \tag{10}$$

Such an approximation has already been used by some authors [11]. Then, the procedure to compute the gradient of the flow equations with respect to the design parameters at constant state (7) will be performed by using the expression presented above (10). In the following sections, this procedure will be first applied to the incompressible Navier-Stokes equations, and then to compressible Euler problems.

3 Incompressible Problems

The incompressible steady-state Navier-Stokes equation may be written as follows:

$$\boldsymbol{R}_u = \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p - \nabla \cdot 2\nu\varepsilon(\boldsymbol{u}), \quad \boldsymbol{R}_p = \nabla \cdot \boldsymbol{u} \quad , \tag{11}$$

plus appropriate boundary conditions. $\boldsymbol{u}$ and p are the velocity and pressure fields, respectively, ν the kinematic viscosity, and $\varepsilon(\cdot)$ is the symmetric gradient of a vector.

Given and objective function I, the continuous adjoint equation for an incompressible flow is expressed as:

$$\begin{aligned} &\int_\Omega \boldsymbol{\psi}^u \cdot (\boldsymbol{u} \cdot \nabla \delta \boldsymbol{u}) + \int_\Omega \boldsymbol{\psi}^u \cdot (\delta \boldsymbol{u} \cdot \nabla \boldsymbol{u}) \\ &+ \int_\Omega \boldsymbol{\psi}^u \cdot (\nabla \delta p) - \int_\Omega \boldsymbol{\psi}^u \cdot \Big(\nabla \cdot (2\nu\varepsilon(\delta\boldsymbol{u}))\Big) \\ &+ \int_\Omega \psi^p \nabla \cdot \delta \boldsymbol{u} + O(\delta \boldsymbol{u}^2) = -\frac{\partial I}{\partial \boldsymbol{u}} \delta \boldsymbol{u} - \frac{\partial I}{\partial p} \delta p \\ &\forall \delta \boldsymbol{u}, \delta p \ \text{ admisible} \quad , \end{aligned} \tag{12}$$

where $\boldsymbol{\psi}^u$ and ψ^p are the adjoint velocity vector and adjoint pressure field, respectively.

Integrating by parts all the terms in equation (12) (the viscous one must be integrated twice), the following expression is obtained (Γ is the boundary of Ω):

$$\begin{aligned} &\int_\Gamma (\boldsymbol{n} \cdot \boldsymbol{u})(\boldsymbol{\psi}^u \cdot \delta \boldsymbol{u}) - \int_\Omega \delta \boldsymbol{u} \cdot (\boldsymbol{u} \cdot \nabla \boldsymbol{\psi}^u) \\ &+ \int_\Gamma (\boldsymbol{n} \cdot \delta \boldsymbol{u})(\boldsymbol{\psi}^u \cdot \boldsymbol{u}) - \int_\Omega \delta \boldsymbol{u} \cdot (\nabla \boldsymbol{\psi}^u \cdot \boldsymbol{u}) \\ &+ \int_\Gamma \delta p \ \boldsymbol{\psi}^u \cdot \boldsymbol{n} - \int_\Omega \delta p \nabla \cdot \boldsymbol{\psi}^u \\ &+ \int_\Gamma \psi^p \boldsymbol{n} \cdot \delta \boldsymbol{u} - \int_\Omega \delta \boldsymbol{u} \cdot \nabla \psi^p \\ &- \int_\Gamma 2\nu \boldsymbol{\psi}^u \cdot \varepsilon(\delta \boldsymbol{u}) \cdot \boldsymbol{n} + \int_\Gamma 2\nu \boldsymbol{n} \cdot \varepsilon(\boldsymbol{\psi}^u) \cdot \delta \boldsymbol{u} \\ &- \int_\Omega \delta \boldsymbol{u} \cdot \nabla \cdot \Big(2\nu\varepsilon(\boldsymbol{\psi}^u)\Big) = \\ &-\frac{\partial I}{\partial \boldsymbol{u}} \delta \boldsymbol{u} - \frac{\partial I}{\partial p} \delta p \ \ \forall \delta \boldsymbol{u}, \delta p \ \text{ admisible} \quad . \end{aligned} \tag{13}$$

Equation (13) is the basis to compute the adjoint velocities and pressures. It is no more than the variational formulation of the following PDE problem for the adjoint variables:

$$-\boldsymbol{u}\cdot\nabla\psi^{u}-\nabla\boldsymbol{\psi}^{u}\cdot\boldsymbol{u}-\nabla\psi^{p}-\nabla\cdot\Big(2\nu\varepsilon(\boldsymbol{\psi}^{u})\Big)$$
$$=\boldsymbol{f}^{u},\quad -\nabla\cdot\psi^{u}=f^{p}\quad\text{in}\quad\Omega \tag{14}$$

plus compatible boundary conditions on Γ. Above, the terms $\boldsymbol{f}^{u}$ and f^{p} will be defined by the partial derivatives of I with respect to $\boldsymbol{u}$ and p in Ω. The boundary conditions will be obtained from the boundary terms in (13), and, as in the domain, by the partial derivatives of I with respect to $\boldsymbol{u}$ and p on Γ. Some examples for different objective functions will be presented later.

At this point, it is important to remark that (13) is obtained by taking a second order approximation of $(\partial\boldsymbol{R}_u/\partial\boldsymbol{u})\delta\boldsymbol{u}$. A first order approximation may be implemented by neglecting the second term of (12), which is $O(\delta\boldsymbol{u})$. In this case, the second term of (14) dissapears, and the adjoint problem will have the same convective diffusive character than the flow one, with the important distinction that it is linear. Some authors take advantage of this feature to use exactly the same numerical technique to solve both the flow and the adjoint problem [3, 12, 1].

Finally, the gradient is obtained from equation (4), and using equations (7) and (10) to approximate $(\partial\boldsymbol{R}/\partial\boldsymbol{\beta})\delta\boldsymbol{\beta}$ as follows:

$$\delta L=\frac{\partial I}{\partial\boldsymbol{\beta}}\delta\boldsymbol{\beta}+\int_{\Omega}\boldsymbol{\psi}^{u}\cdot\boldsymbol{u}\cdot\nabla\delta\boldsymbol{u}+\int_{\Omega}\boldsymbol{\psi}^{u}\cdot\delta\boldsymbol{u}\cdot\nabla\boldsymbol{u}$$
$$+\int_{\Omega}\boldsymbol{\psi}^{u}\cdot\delta\boldsymbol{u}\cdot\nabla\delta\boldsymbol{u}+\int_{\Omega}\psi^{u}\cdot\nabla\delta p$$
$$-\int_{\Omega}\boldsymbol{\psi}^{u}\cdot\nabla\cdot\Big(2\nu\varepsilon(\delta\boldsymbol{u})\Big)+\int_{\Omega}\psi^{p}\nabla\cdot\delta\boldsymbol{u}\quad. \tag{15}$$

Neglecting the second order term (fourth right hand side term), and integrating by parts as in (12), the following expression is obtained:

$$\delta L=\frac{\partial I}{\partial\boldsymbol{\beta}}\delta\boldsymbol{\beta}+\int_{\Gamma}(\boldsymbol{n}\cdot\boldsymbol{u})(\boldsymbol{\psi}^{u}\cdot\delta\boldsymbol{u})-\int_{\Omega}\delta\boldsymbol{u}\cdot(\boldsymbol{u}\cdot\nabla\psi^{u})$$
$$+\int_{\Gamma}(\boldsymbol{n}\cdot\delta\boldsymbol{u})(\boldsymbol{\psi}^{u}\cdot\boldsymbol{u})-\int_{\Omega}\delta\boldsymbol{u}\cdot(\nabla\boldsymbol{\psi}^{u}\cdot\boldsymbol{u})$$
$$+\int_{\Gamma}\delta p\,\boldsymbol{\psi}^{u}\cdot\boldsymbol{n}-\int_{\Omega}\delta p\nabla\cdot\boldsymbol{\psi}^{u}+\int_{\Gamma}\psi^{p}\boldsymbol{n}\cdot\delta\boldsymbol{u}$$
$$-\int_{\Omega}\delta\boldsymbol{u}\cdot\nabla\psi^{p}-\int_{\Gamma}2\nu\boldsymbol{\psi}^{u}\cdot\varepsilon(\delta\boldsymbol{u})\cdot\boldsymbol{n}$$
$$+\int_{\Gamma}2\nu\boldsymbol{n}\cdot\varepsilon(\boldsymbol{\psi}^{u})\cdot\delta\boldsymbol{u}-\int_{\Omega}\delta\boldsymbol{u}\cdot\nabla\cdot\Big(2\nu\varepsilon(\boldsymbol{\psi}^{u})\Big)\quad. \tag{16}$$

The above equation is the key to compute the required sensitivities. For most objective functions, as it will be shown later, the domain terms are exactly canceled: They will fulfill the adjoint PDE problem (equations (14)). This point will be clarified in the next sections.

3.1 Gradient of Total Forces

To compute the gradient of a force over a given surface $\mathcal{S}$, the following objective function may be defined:

$$I=\int_{\mathcal{S}}-\boldsymbol{n}\cdot\Big(2\nu\varepsilon(\boldsymbol{u})-p\boldsymbol{I}\Big)\cdot\boldsymbol{d}\quad, \tag{17}$$

where $\boldsymbol{n}$ is the exterior normal to the flow domain Ω, and $\boldsymbol{d}$ is the force direction (i.e. drag or lift direction). The variation of I with respect to the flow variables at fixed domain is given by:

$$\frac{\partial I}{\partial\boldsymbol{u}}\delta\boldsymbol{u}+\frac{\partial I}{\partial p}\delta p=-\int_{\mathcal{S}}\boldsymbol{n}\cdot 2\nu\varepsilon(\delta\boldsymbol{u})\cdot\boldsymbol{d}+\int_{\mathcal{S}}\boldsymbol{n}\cdot\boldsymbol{d}\,\delta p\quad. \tag{18}$$

By replacing this expressions in (13), the following continuous adjoint problem can be written:

$$\begin{aligned}&-\boldsymbol{u}\cdot\nabla\psi^{u}-\nabla\boldsymbol{\psi}^{u}\cdot\boldsymbol{u}-\nabla\psi^{p}-\nabla\cdot\Big(2\nu\varepsilon(\boldsymbol{\psi}^{u})\Big)=\boldsymbol{0}\\&-\nabla\cdot\psi^{u}=0\quad\text{in}\quad\Omega\\&\boldsymbol{\psi}^{u}=-\boldsymbol{d}\quad\text{on}\quad\mathcal{S},\quad\boldsymbol{\psi}^{u}=\boldsymbol{0}\quad\text{on}\quad\Gamma_{\text{out}},\\&\boldsymbol{n}\cdot\varepsilon(\boldsymbol{\psi}^{u})=\boldsymbol{0}\quad\text{on}\quad\Gamma_{\text{in}}\quad.\end{aligned} \tag{19}$$

The above set of boundary conditions exactly cancels all the boundary terms of equation (13). This is: $\delta\boldsymbol{u}=\boldsymbol{0}$ on $\mathcal{S}$ and on the outflow (Γ_{out}) ($\delta\boldsymbol{u}$ is the test function associated to the adjoint velocity, then it is zero wherever $\boldsymbol{\psi}^{u}$ is prescribed). At the inflow (Γ_{in}) the normal adjoint velocity gradient is zero, and $\delta\boldsymbol{u}=0$ if Γ_{in} is far enough from $\mathcal{S}$. The rest of boundary terms are automatically fulfilled by the election of $\boldsymbol{\psi}^{u}$ on $\mathcal{S}$.

Obtained $\boldsymbol{\psi}^{u}$ and ψ^{p} by solving the above PDE problem, the gradient of the objective function is easily computed by equation (16). In such an expression, all the domain terms are eliminated (they exactly fulfill the adjoint problem), and the gradient may be computed by using only the boundary terms and the approximation to $\delta\boldsymbol{u}$ and δp given by (10) as follows:

$$\frac{\delta L}{\delta\boldsymbol{\beta}}=\frac{\partial I}{\partial\boldsymbol{\beta}}-\int_{\mathcal{S}}(\nabla p\cdot\boldsymbol{n})(\boldsymbol{\psi}^{u}\cdot\boldsymbol{n})-\int_{\mathcal{S}}\psi^{p}\boldsymbol{n}\cdot(\nabla\boldsymbol{u}\cdot\boldsymbol{n})$$
$$+\int_{\mathcal{S}}2\nu\boldsymbol{\psi}^{u}\cdot\varepsilon(\boldsymbol{n}\cdot\nabla\boldsymbol{u})\cdot\boldsymbol{n}$$
$$-\int_{\mathcal{S}}2\nu(\boldsymbol{n}\cdot\varepsilon(\boldsymbol{\psi}^{u}))\cdot(\nabla\boldsymbol{u}\cdot\boldsymbol{n})\quad. \tag{20}$$

In this last expression, it was assumed that the gradients of $\boldsymbol{u}$ and p are zero at Γ_{in} and Γ_{out}. Therefore, by (10), $\delta\boldsymbol{u} = \mathbf{0}$ and $\delta p = 0$ at those parts of the boundary. Again, the term $\partial I/\partial\boldsymbol{\beta}$ which is the geometric part of the gradient may be easily computed in an exact analitical way, or by finite differences. The computation of the sensitivities using only the solution of the flow and adjoint on the boundary, has been already carried out by some authors [1, 11, 6]. The expressions presented below, equations (16) and (20), can be seen as generalization of such a procedure.

At this point, it is important to remark that two levels of incomplete gradient may be used to avoid the solution of the adjoint problem. The first one is to take only the geometric part of the gradient (first term of (20)) [10, 11]. The second one is obtained by neglecting the terms involving ψ^p and the gradients of $\boldsymbol{\psi}^u$ [23, 22] ($\boldsymbol{\psi}^u \cdot \boldsymbol{n}$ is known at $\mathcal{S}$ from the boundary conditions). Then, the incomplete gradient could be written as:

$$\frac{\delta L}{\delta\boldsymbol{\beta}} \approx \frac{\partial I}{\partial\boldsymbol{\beta}} - \int_{\mathcal{S}} (\nabla p \cdot \boldsymbol{n})(\boldsymbol{\psi}^u \cdot \boldsymbol{n}) - \int_{\mathcal{S}} 2\nu\boldsymbol{\psi}^u \cdot \varepsilon(\boldsymbol{n}\cdot\nabla\boldsymbol{u})\cdot\boldsymbol{n} \quad . \tag{21}$$

It can be noticed that such an approximation may not be good for viscous problems, because the terms involving ψ^p and $\varepsilon(\boldsymbol{\psi}^u)$ may be important (third and last terms of (20)). However, for Euler problems ($\nu = 0$), the only term that is neglected is the third one, which involves the normal component of the velocity gradient at $\mathcal{S}$. Such a term is close to zero in most cases.

Another important remark is that the gradient equation (16), could be also obtained by taking into account that the total variation of $\boldsymbol{R}$ must be zero. This is:

$$\delta\boldsymbol{R} = \frac{\partial\boldsymbol{R}}{\partial\boldsymbol{\beta}}\delta\boldsymbol{\beta} + \frac{\partial\boldsymbol{R}}{\partial\boldsymbol{U}}\delta\boldsymbol{U} = \mathbf{0} \quad . \tag{22}$$

Hence, $(\partial\boldsymbol{R}/\partial\boldsymbol{\beta})\delta\boldsymbol{\beta}$ in (7) could be replaced by $-(\partial\boldsymbol{R}/\partial\boldsymbol{U})\delta\boldsymbol{U}$. This procedure leads to exactly the same results obtained in this section.

4 Compressible Euler Problems

The set of equations that governs non-viscous steady-state compressible flow problems can be written as:

$$\boldsymbol{R}_\rho = \nabla\cdot(\rho\boldsymbol{u}) = 0,$$
$$\boldsymbol{R}_u = \nabla\cdot\Big(\rho(\boldsymbol{u}\otimes\boldsymbol{u})\Big) + \nabla p = 0, \quad \text{and}$$
$$\boldsymbol{R}_e = \nabla\cdot\Big(\boldsymbol{u}(\rho e + p)\Big) = 0 \quad \text{in} \quad \Omega \quad . \tag{23}$$

where ρ is the density of the fluid and e the specific energy (the rest of variables have been already defined). The above set of PDE must be closed with compatible boundary conditions, and with a state equation to relate the pressure with the other variables (density, energy and velocities). In this work, the polytropic gas equation is chosen:

$$p = (\gamma - 1)\rho(e - \frac{1}{2}\boldsymbol{u}^2) \quad , \tag{24}$$

where γ is the ratio of specific heats (1.4 for most gases). As in the previous section, the adjoint equation is obtained by introducing the adjoint variables (ψ^ρ, $\boldsymbol{\psi}^u$, ψ^e), by approximating $(\partial\boldsymbol{R}/\partial\boldsymbol{U})\delta\boldsymbol{U}$ to second order (terms of $O(\delta\boldsymbol{U}^2)$ are neglected), and by integrating by parts. This is:

$$\begin{aligned}
&\int_\Gamma (\boldsymbol{n}\cdot\boldsymbol{u})\psi^\rho\delta\rho - \int_\Omega \delta\rho\boldsymbol{u}\cdot\nabla\psi^\rho + \int_\Gamma (\delta\boldsymbol{u}\cdot\boldsymbol{n})\rho\psi^\rho \\
&- \int_\Omega \rho\delta\boldsymbol{u}\cdot\nabla\psi^\rho + \int_\Gamma \delta\rho(\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^u\cdot\boldsymbol{u}) \\
&- \int_\Omega \delta\rho\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^u\cdot\boldsymbol{u} + \int_\Gamma \rho(\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^u\cdot\delta\boldsymbol{u}) \\
&- \int_\Omega \rho\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^u\cdot\delta\boldsymbol{u} + \int_\Gamma \rho(\delta\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^u\cdot\boldsymbol{u}) \\
&- \int_\Omega \rho\delta\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^u\cdot\boldsymbol{u} + \int_\Gamma (\boldsymbol{\psi}^u\cdot\boldsymbol{n})(\gamma-1)\delta\rho(e - \frac{\boldsymbol{u}^2}{2}) \\
&+ \int_\Gamma (\boldsymbol{\psi}^u\cdot\boldsymbol{n})(\gamma-1)\rho(\delta e - \boldsymbol{u}\cdot\delta\boldsymbol{u}) \\
&- \int_\Omega \delta\rho(\gamma-1)(e - \frac{\boldsymbol{u}^2}{2})\nabla\cdot\boldsymbol{\psi}^u \\
&- \int_\Omega \rho(\gamma-1)(\delta e - \boldsymbol{u}\cdot\delta\boldsymbol{u})\nabla\cdot\boldsymbol{\psi}^u \\
&+ \int_\Gamma (\delta\boldsymbol{u}\cdot\boldsymbol{n})\psi^e\Big(\rho e + (\gamma-1)\rho(e - \frac{\boldsymbol{u}^2}{2})\Big) \\
&- \int_\Omega \delta\boldsymbol{u}\cdot\nabla\psi^e\Big(\rho e + (\gamma-1)\rho(e - \frac{\boldsymbol{u}^2}{2})\Big) \\
&+ \int_\Gamma (\boldsymbol{u}\cdot\boldsymbol{n})\psi^e\Big(\rho\delta e + e\delta\rho + (\gamma-1)\delta\rho(e - \frac{\boldsymbol{u}^2}{2}) \\
&+ (\gamma-1)\rho(\delta e - \boldsymbol{u}\cdot\delta\boldsymbol{u})\Big) - \int_\Omega \boldsymbol{u}\cdot\nabla\psi^e\Big(\rho\delta e + e\delta\rho \\
&+ (\gamma-1)\delta\rho(e - \frac{\boldsymbol{u}^2}{2}) + (\gamma-1)\rho(\delta e - \boldsymbol{u}\cdot\delta\boldsymbol{u})\Big) \\
&= -\frac{\partial I}{\partial\boldsymbol{U}_k}\delta\boldsymbol{U}_k \quad \forall\delta\rho, \delta\boldsymbol{u}, \delta e \ \text{ admisibles} \ ,
\end{aligned} \tag{25}$$

where $(U_1, U_2, U_3, U_4, U_5)$ are (ρ, u_1, u_2, u_3, e) respectively. The previous expression is nothing more than the variational form of the following strong PDE problem:

$$
\begin{aligned}
&-\boldsymbol{u}\cdot\nabla\psi^{\rho}-\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^{u}\cdot\boldsymbol{u}-(\gamma-1)(e-\frac{u^2}{2})\\
&\nabla\cdot\boldsymbol{\psi}^{u}-\boldsymbol{u}\cdot\nabla\psi^{e}\Big(e+(\gamma-1)(e-\frac{u^2}{2})\Big)=f^{\rho}\\
&-\rho\nabla\psi^{\rho}-\rho\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^{u}-\rho\nabla\boldsymbol{\psi}^{u}\cdot\boldsymbol{u}+(\gamma-1)\rho\boldsymbol{u}(\nabla\cdot\boldsymbol{\psi}^{u})\\
&-\nabla\psi^{e}\Big(\rho e+(\gamma-1)\rho(e-\frac{u^2}{2})\Big)+\boldsymbol{u}\cdot\nabla\psi^{e}(\gamma-1)\rho\boldsymbol{u}\\
&=\boldsymbol{f}^{u} \qquad (26)\\
&-(\gamma-1)\rho(\nabla\cdot\boldsymbol{\psi}^{u})-\boldsymbol{u}\cdot\nabla\psi^{e}(\rho+(\gamma-1)\rho)=f^{e}
\end{aligned}
$$

where f^{ρ}, $\boldsymbol{f}^{u}$ and f^{e} will be defined by the partial derivatives of I with respect to ρ, $\boldsymbol{u}$ and e in Ω. The boundary conditions will be obtained from the boundary terms in (25), and, as in the domain, by the partial derivatives of I with respect to the flow variables (ρ, $\boldsymbol{u}$ and e) in Γ. Examples for different objective functions will be presented later.

Although easy, but very tedious (the authors already did it), one may check that: If the flow equations (23) are written in the well known advective form,

$$\boldsymbol{A}_k\frac{\partial\boldsymbol{U}_k}{\partial x_k}=0, \qquad (27)$$

where $\boldsymbol{A}_k,\quad k=1,2,3$ are the 5×5 advective matrices, the adjoint problem (26) may be expressed as:

$$-\boldsymbol{A}_k^T\frac{\partial\boldsymbol{\Psi}_k}{\partial x_k}=\boldsymbol{F}, \qquad (28)$$

where $\boldsymbol{A}_k^T$ is the transpose of $\boldsymbol{A}_k$. This fact is exploited for some authors to use the same numerical technique for solving both, the flow and the adjoint problems [3, 12, 1].

As in the incompressible case, the gradient of the objective function with respect to the design parameters is computed by using the approximations to $(\partial\boldsymbol{R}/\partial\boldsymbol{\beta})\cdot\delta\boldsymbol{\beta}$ and to $\delta\boldsymbol{U}_k$ presented in equations (7)-(10):

$$
\begin{aligned}
\delta L=&\frac{\partial I}{\partial\boldsymbol{\beta}}\delta\boldsymbol{\beta}+\int_{\Gamma}(\boldsymbol{n}\cdot\boldsymbol{u})\psi^{\rho}\delta\rho-\int_{\Omega}\delta\rho\boldsymbol{u}\cdot\nabla\psi^{\rho}\\
&+\int_{\Gamma}(\delta\boldsymbol{u}\cdot\boldsymbol{n})\rho\psi^{\rho}-\int_{\Omega}\rho\delta\boldsymbol{u}\cdot\nabla\psi^{\rho}\\
&+\int_{\Gamma}\delta\rho(\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^{u}\cdot\boldsymbol{u})-\int_{\Omega}\delta\rho\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^{u}\cdot\boldsymbol{u}\\
&+\int_{\Gamma}\rho(\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^{u}\cdot\delta\boldsymbol{u})-\int_{\Omega}\rho\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^{u}\cdot\delta\boldsymbol{u}\\
&+\int_{\Gamma}\rho(\delta\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^{u}\cdot\boldsymbol{u})-\int_{\Omega}\rho\delta\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}^{u}\cdot\boldsymbol{u}\\
&+\int_{\Gamma}(\boldsymbol{\psi}^{u}\cdot\boldsymbol{n})(\gamma-1)\delta\rho(e-\frac{\boldsymbol{u}^2}{2})\\
&+\int_{\Gamma}(\boldsymbol{\psi}^{u}\cdot\boldsymbol{n})(\gamma-1)\rho(\delta e-\boldsymbol{u}\cdot\delta\boldsymbol{u})\\
&-\int_{\Omega}\delta\rho(\gamma-1)(e-\frac{\boldsymbol{u}^2}{2})\nabla\cdot\boldsymbol{\psi}^{u}\\
&-\int_{\Omega}\rho(\gamma-1)(\delta e-\boldsymbol{u}\cdot\delta\boldsymbol{u})\nabla\cdot\boldsymbol{\psi}^{u}\\
&+\int_{\Gamma}(\delta\boldsymbol{u}\cdot\boldsymbol{n})\psi^{e}\Big(\rho e+(\gamma-1)\rho(e-\frac{\boldsymbol{u}^2}{2})\Big)\\
&-\int_{\Omega}\delta\boldsymbol{u}\cdot\nabla\psi^{e}\Big(\rho e+(\gamma-1)\rho(e-\frac{\boldsymbol{u}^2}{2})\Big)\\
&+\int_{\Gamma}(\boldsymbol{u}\cdot\boldsymbol{n})\psi^{e}\Big(\rho\delta e+e\delta\rho+(\gamma-1)\delta\rho(e-\frac{\boldsymbol{u}^2}{2})\\
&+(\gamma-1)\rho(\delta e-\boldsymbol{u}\cdot\delta\boldsymbol{u})\Big)\\
&-\int_{\Omega}\boldsymbol{u}\cdot\nabla\psi^{e}\Big(\rho\delta e+e\delta\rho+(\gamma-1)\delta\rho(e-\frac{\boldsymbol{u}^2}{2})\\
&+(\gamma-1)\rho(\delta e-\boldsymbol{u}\cdot\delta\boldsymbol{u})\Big) \qquad (29)
\end{aligned}
$$

Again, the above equation is the key to compute the required sensitivities for compressible Euler problems. As it will be shown in the following section, for most objective functions the domain terms are exactly canceled: They will fulfill the adjoint PDE problem (equation (26)). Therefore, the gradient is computed by using only the remaining boundary terms.

4.1 Gradient of Non-viscous Forces

As for the incompressible viscous flows, the objective function to compute the gradient of some force over a given surface $\mathcal{S}$ is defined by:

$$I=\int_{\mathcal{S}}\boldsymbol{n}\cdot\boldsymbol{d}\ p\quad , \qquad (30)$$

where $\boldsymbol{n}$ is the exterior normal to the flow domain Ω, and $\boldsymbol{d}$ is the force direction (i.e. drag or lift direction). The variation of I with respect to the flow variables at fixed domain is given by:

$$\frac{\partial I}{\partial p}\ \delta p=\int_{\mathcal{S}}\boldsymbol{n}\cdot\boldsymbol{d}\ \delta p\quad . \qquad (31)$$

The adjoint problem associated to the previous objective function is given by (26), taking $f^{p}=0$, $\boldsymbol{f}^{u}=\boldsymbol{0}$ and $f^{e}=0$. To obtain the right boundary conditions, it is better to write the remaining terms of (25) (all the domain terms are automatically canceled due to the solution of the adjoint problem into the flow domain), in terms of δp. This is done via the second order variation of the state equation:

$$\delta p = (\gamma - 1)\delta\rho(e - \frac{\boldsymbol{u}^2}{2}) + (\gamma - 1)\rho(\delta e - \boldsymbol{u}\cdot\delta\boldsymbol{u}) \quad , \quad (32)$$

as follows:

$$\begin{aligned}&\int_\Gamma (\boldsymbol{n}\cdot\boldsymbol{u})\psi^\rho\delta\rho + \int_\Gamma(\delta\boldsymbol{u}\cdot\boldsymbol{n})\rho\psi^\rho \\ &+\int_\Gamma \delta\rho(\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^u\cdot\boldsymbol{u}) + \int_\Gamma \rho(\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^u\cdot\delta\boldsymbol{u}) \\ &+\int_\Gamma \rho(\delta\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^u\cdot\boldsymbol{u}) + \int_\Gamma(\boldsymbol{\psi}^u\cdot\boldsymbol{n})\ \delta p \\ &+\int_\Gamma(\delta\boldsymbol{u}\cdot\boldsymbol{n})\psi^e(\rho e + p) + \int_\Gamma(\boldsymbol{u}\cdot\boldsymbol{n})\psi^e \\ &(\rho\delta e + e\delta\rho + \delta p) = -\int_{\mathcal{S}} \boldsymbol{n}\cdot\boldsymbol{d}\ \delta p \quad . \qquad (33)\end{aligned}$$

If $\boldsymbol{\psi}^u\cdot\boldsymbol{n} = -\boldsymbol{d}\cdot\boldsymbol{n}$ on $\mathcal{S}$ is chosen, $\delta\boldsymbol{u}\cdot\boldsymbol{n}$ is automatically zero on $\mathcal{S}$. In addition, $\boldsymbol{u}\cdot\boldsymbol{n} = \boldsymbol{0}$ on $\mathcal{S}$, and taking the inflow and outflow far enough to assume that $\delta\rho = 0$, $\delta e = 0$ and $\delta\boldsymbol{u} = \boldsymbol{0}$, (33) is satisfied. Actually, all the adjoint variables can be prescribed at inflow and outflow in such a way that the advective problem is well posed.

Then, given the values for $\boldsymbol{\Psi}$, the gradient is computed by the following espression (using (29) and introducing (10)):

$$\begin{aligned}&\frac{\delta L}{\delta\beta} = \frac{\partial I}{\partial\beta} - \int_{\mathcal{S}}(\boldsymbol{n}\cdot\nabla\boldsymbol{u}\cdot\boldsymbol{n})\rho\psi^\rho \\ &-\int_{\mathcal{S}}\rho(\boldsymbol{n}\cdot\nabla\boldsymbol{u}\cdot\boldsymbol{n})(\boldsymbol{\psi}^u\cdot\boldsymbol{u}) - \int_{\mathcal{S}}(\boldsymbol{\psi}^u\cdot\boldsymbol{n})\ \boldsymbol{n}\cdot\nabla p \\ &-\int_{\mathcal{S}}(\boldsymbol{n}\cdot\nabla\boldsymbol{u}\cdot\boldsymbol{n})\psi^e(\rho e + p) \quad . \qquad (34)\end{aligned}$$

Therefore, the gradient is computed by using only the flow and adjoint solutions on $\mathcal{S}$. An incomplete gradient can be computed by using the terms of (34) that are already known before solving the adjoint problem. These are:

$$\begin{aligned}\frac{\delta L}{\delta\beta} &\approx \frac{\partial I}{\partial\beta} - \int_{\mathcal{S}}(\boldsymbol{\psi}^u\cdot\boldsymbol{n})\ \boldsymbol{n}\cdot\nabla p \\ &= \frac{\partial I}{\partial\beta} - \int_{\mathcal{S}}(\boldsymbol{d}\cdot\boldsymbol{n})\frac{\partial p}{\partial\boldsymbol{n}} \quad . \qquad (35)\end{aligned}$$

Finally, it is important to remark that expression (35), is a very good approximation to the gradient for problems where the normal velocity gradient at $\mathcal{S}$ is close to zero (all the neglected terms of (34) are multiplied by $\partial\boldsymbol{u}/\partial\boldsymbol{n}\cdot\boldsymbol{n}$).

REMARK: The expressions for the gradient (left hand side of (33)) can also be obtained by using the well known form for the steady-state Euler equations: $\nabla\cdot\boldsymbol{F} = \boldsymbol{0}$. This is:

$$\int_\Omega \boldsymbol{\Psi}\cdot\frac{\partial\boldsymbol{R}}{\partial\boldsymbol{x}}\delta\boldsymbol{x} = -\int_\Omega \psi_l\cdot\frac{\partial\delta F_l^k}{\partial x_k}$$
$$\text{for } \ l = 1,...,n_\text{d}+2 \ \text{ and } \ k = 1,...,n_\text{d} \quad , \quad (36)$$

where n_d is the spatial dimension of the problem. Integrating by parts, the following is obtained:

$$\int_\Omega \frac{\partial\psi_l}{\partial x_k}\delta F_l^k - \int_\Gamma \psi_l\delta F_l^k n_k = 0 \quad . \qquad (37)$$

Now, δF_l^k may be approximated by its Taylor's expansion:

$$F_l^k(\boldsymbol{x}+\epsilon\boldsymbol{e}^m) = F_l^k(\boldsymbol{x}) + \epsilon\boldsymbol{e}^m\cdot\frac{\partial F_l^k}{\partial\boldsymbol{x}} \quad , \qquad (38)$$

where $0 < \epsilon << 1$, and $\boldsymbol{e}^m$ is the global direction m. Assuming that the domain part of (37) is zero due to the solution of the adjoint problem, the following general expression can be written for (36):

$$\int_\Omega \psi_l\frac{\partial\boldsymbol{R}_l}{\partial x_m}\delta x_m = -\int_\Gamma \psi_l\frac{\partial F_l^k}{\partial x_m}n_k \quad . \qquad (39)$$

This will be the expression to obtain the adjoint part of the gradient in the global direction m. It is easy to check (but very tedious) that if the direction $\boldsymbol{e}^m$ is replaced by the exterior normal $\boldsymbol{n}$, the left hand side of (33) is obtained.

5 Geometric Constraints

Given a objective function, the gradients are computed using the expressions previously developed (see equations (20) and (34)). Then, the geometric constraints (maximum thickness, etc,) are imposed using an improved pseudo-shell approach. A former version of such a scheme can be consulted in [26]. The procedure is as follows.

Assume that a finite element discretization of a surface $\mathcal{S}$, support of some objective function L, is given. Assume that the movement x_k^i $(k = 1,2,3)$ of every node i on $\mathcal{S}$ is taken as a design parameter. If the gradient of L with respect to each of such a design parameters $(\partial L/\partial x_k^i)$ is obtained, (i.e. by an adjoint formulation, finite differences, a direct method, etc,) the following PDE problem can be defined: Find the displacement ($\boldsymbol{u}$) and rotation ($\boldsymbol{\theta}$) fields on $\mathcal{S}$ such that,

$$
\begin{aligned}
&\theta_l - \frac{\partial u_n}{\partial \boldsymbol{t}^l} = 0 \ ; \ \theta_n = 0 \ ; \\
&u_n + \frac{\partial}{\partial \boldsymbol{t}^l}\Big(\theta_l - \tau \frac{\partial u_n}{\partial \boldsymbol{t}^l}\Big) = \frac{\partial L}{\partial \boldsymbol{n}} \ ; \\
&u_l + \frac{\partial}{\partial \boldsymbol{t}^k}\Big[\mu\Big(\frac{\partial u_l}{\partial \boldsymbol{t}^k} + \frac{\partial u_k}{\partial \boldsymbol{t}^l}\Big)\Big] \\
&+ \frac{\partial}{\partial \boldsymbol{t}^l}\Big[\Big(\frac{\mu\gamma}{1-2\gamma}\Big)\frac{\partial u_k}{\partial \boldsymbol{t}^k}\Big] = \frac{\partial L}{\partial \boldsymbol{t}^l}
\end{aligned} \tag{40}
$$

for $l,k = 1,2$. Above $\boldsymbol{n}$ is the normal, $\boldsymbol{t}^1$ the first tangent vector and $\boldsymbol{t}^2$ the second tangent vector, which span a local orthonormal basis on every point of $\mathcal{S}$; u_n, u_1 and u_2 are the displacement components on such a basis; and θ_n, θ_1 and θ_2 are the components of the rotation vector. The boundary conditions of the pseudo-shell equations ((40)) are given by a subset of the geometric constraints of the optimization problem (i.e. a set of points i are allowed to move only in an specific direction, and/or some rotations are set to zero). The constants μ and γ have the physical meaning of the material shear modul and the Poisson ratio, respectively. τ is the stabilization parameter (see [26]).

The above PDE problem is solved by using linear finite elements (P1), equal order interpolation for both fields ($\boldsymbol{u}$ and $\boldsymbol{\theta}$), and the stabilized finite element formulation presented in [26]. The final displacement field is scaled to fulfill a maximum allowed displacement defined by the user (i.e. some average size of the elements on $\mathcal{S}$).

The improvement with respect to the scheme presented in [26], is that the sensitivities $\partial L/\partial \boldsymbol{x}$ are applied as sources to the PDE problem, instead of as boundary conditions. Such a change allows to re-use the LU decomposition matrices for enforcing some geometric constraints in a very fast manner (the discretized counterpart of (1) is solved using a LU direct solver and the L and U matrices are stored). This new feature is illustrated by the following algorithm, which describes how a minimum thickness field ($t_{\min}(\boldsymbol{x})$) may be enforced on $\mathcal{S}$:

Algorithm 1

1 Continuation-flag$\leftarrow 0$

Do $i = 1$, number of nodes on $\mathcal{S}$

Obtain $\boldsymbol{x}'^i = \boldsymbol{x}^i - \boldsymbol{u}^i$

If $\Big((y^i - \boldsymbol{x}'^i)\cdot \boldsymbol{n}^i < t(\boldsymbol{x}^i)\Big)$ **then**

- Continuation-flag=1
- Compute $\boldsymbol{u}'^i$ such that: $\Big(y^i - (\boldsymbol{x}^i - (\boldsymbol{u}^i + \boldsymbol{u}'^i))\Big)\cdot \boldsymbol{n}^i = t(\boldsymbol{x}^i)$
- Redefine $\partial L/\partial \boldsymbol{x}^i \leftarrow \boldsymbol{u}^i + \boldsymbol{u}'^i$

End if

End Do

If (Continuation-flag=1) **then**

- Solve pseudo-shell problem to obtain a new displacement field ($\boldsymbol{u}$). Only a very fast backward and forward substitution is required due to the storage of the LU matrices.
- Goto **1**

Else finish

Above, $\boldsymbol{x}^i$ and $\boldsymbol{x}'^i$ are the old and new positions of the nodal point i, $\boldsymbol{u}^i$ is its scaled displacement (in the direction of the gradient due to the solution of (1), and after it is scaled to fit a maximum allowed movement), $\boldsymbol{n}^i$ is the external normal on i, and y^i is the intersection point between the vector defined by $\boldsymbol{x}^i + \boldsymbol{n}^i$ (and which starts on i) and the surface $\mathcal{S}$.

Finally, The interior mesh is modified using the level approach presented in [25].

6 Numerical Examples

In this section two numerical examples are shown. The first of them is an incompressible Navier-Stokes control problem, and the second one a compressible shape design problem. More numerical examples will be presented in the final version of the paper.

6.1 Lift Control over a Cylinder

A circular cylinder is immersed in a viscous fluid. The *Re* number is based on the diameter and the prescribed inflow velocity. The mesh and geometry are shown in Figure 1. The flow domain is the rectangle $[-3,-5]\times[12,5]$ minus the circle of diameter 1.0 and center coordinates $[0,0]$. Here, the $Re = 100$ standard case is considered.

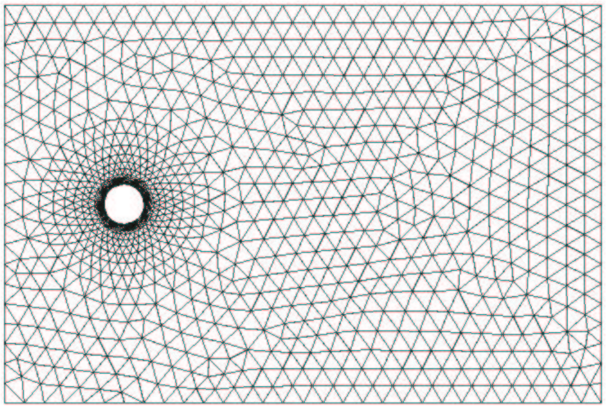

Figure 1: Mesh of 3636 nodes and 1888 linear elements.

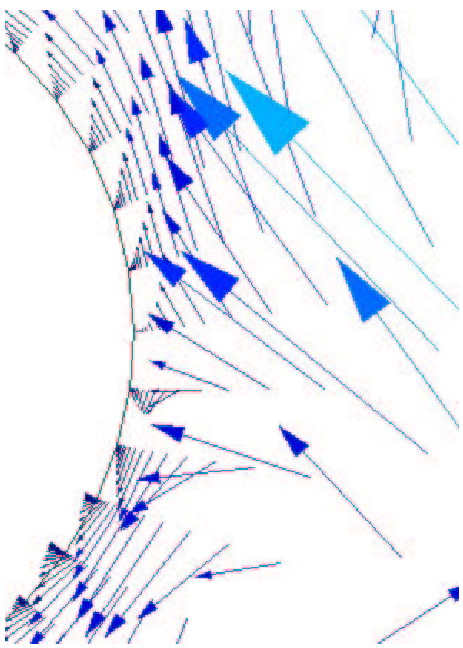

Figure 2: Position of the design parameters (injection velocity): The 3 nodes at the bottom and the 3 top ones.

The control problem consist of minimizing the amplitude of the periodic pressure lift force on the cylinder, by moving a portion of the cylinder surface $\mathcal{S}$ in each time step, or, instead of that, by imposing an equivalent injection velocity (see equation (43) below). The control algorithm is as follows: In each time step, the incomplete gradient of the lift force on the cylinder is computed by equation (21) (the viscous term is neglected because it involves second derivatives at $\mathcal{S}$ which are not well approximated by linear elements), and the control mechanism is applied over the design variables. The design variables are the normal

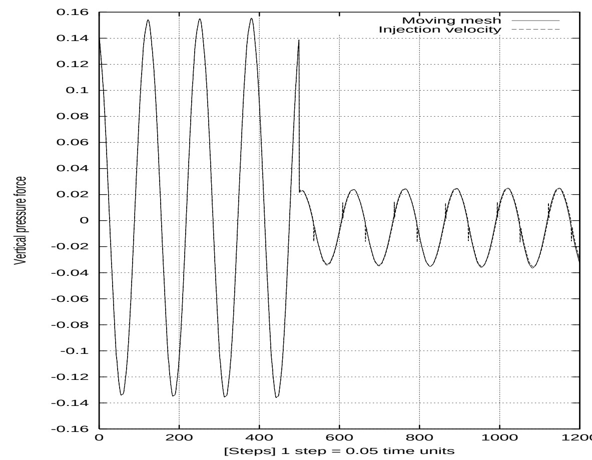

Figure 3: Vertical pressure force evolution before and after the control is applied. Control starts at 500 time steps.

direction of some nodal points behind the cylinder (see Figure 2). The steepest descendent parameter to move the mesh (or to apply the equivalent injection velocity) is the time step size ($\delta t = 0.05$ time units for this case).

The injection velocity is the velocity that has to be applied on the control surface at time $n+1$ ($\boldsymbol{u}^{n+1}$) to decrease the lift force without moving the cylinder surface. Its expression may be obtained from the following Taylor's expansion (see [11]):

$$\begin{aligned} \boldsymbol{v}^{n+1} \cdot \boldsymbol{n}' &= \boldsymbol{u}^{n+1} \cdot \boldsymbol{n} + \boldsymbol{u}^{n} \cdot (\boldsymbol{n}' - \boldsymbol{n}) \\ &+ (\boldsymbol{u}^{n+1} - \boldsymbol{u}^{n}) \cdot \boldsymbol{n} + O(\delta \boldsymbol{u}^2, \delta \boldsymbol{n}^2) \quad , \end{aligned} \tag{41}$$

where the superscripts refer to the time step, $\boldsymbol{v}$ is the velocity on the configuration at time step $n+1$ if the mesh were moving, and $\boldsymbol{u}$ is the velocity on the fixed configuration. $\boldsymbol{n}$ and $\boldsymbol{n}'$ are the exterior normals at the fixed configuration and at the new configuration, respectively.

If it is assumed that the geometry change (change in normals) is more important than the state change (change in velocities), the third RHS term of (41) can be neglected. Moreover, the velocity $\boldsymbol{v}^{n+1}$ that has to be applied over the control surface if the mesh were moving (and using an ALE formulation) is given by:

$$\boldsymbol{v}^{n+1} = \frac{\boldsymbol{x}^{n+1} - \boldsymbol{x}^{n}}{\delta t} \quad , \tag{42}$$

where $\boldsymbol{x}$ is the position vector of the nodes that would be moved. Therefore, the injection velocity ($\boldsymbol{u}^{n+1} \cdot \boldsymbol{n}$) can be obtained as:

$$\boldsymbol{u}^{n+1} \cdot \boldsymbol{n} = \frac{\boldsymbol{x}^{n+1} - \boldsymbol{x}^{n}}{\delta t} \cdot \boldsymbol{n}' - \boldsymbol{u}^{n} \cdot (\boldsymbol{n}' - \boldsymbol{n}) \quad . \tag{43}$$

In Figure 3 the evolution of the lift is presented. The control start to be applied at $t = 25$ (500 time steps). The amplitude of the force is reduced in a 87% for both type of controls. In addition, it can be noticed that the effect of moving the mesh and of applying the injection velocity is exactly the same. The maximum injection velocity was around 1% of the inflow velocity.

6.2 Design of a 3D wing

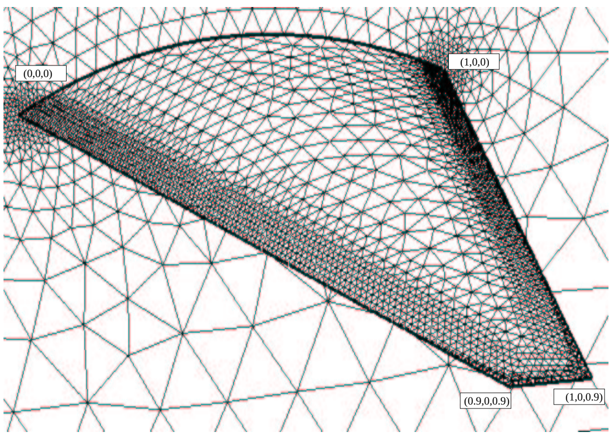

Figure 4: Initial geometry and surface mesh on the wing ($\mathcal{S}$) (3575 nodal points). The corner coordinate values are also shown

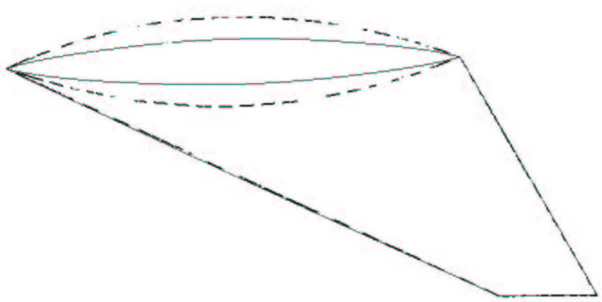

Figure 5: Initial (dashed line) and final (continuous line) geometries. A small twist at the final geometry can be noticed

To illustrate how the pseudo-shell approach works, the drag force (C_d) at constant lift (C_l) over a hypersonic wing (at a angle of attack of 5º degress) was optimized,

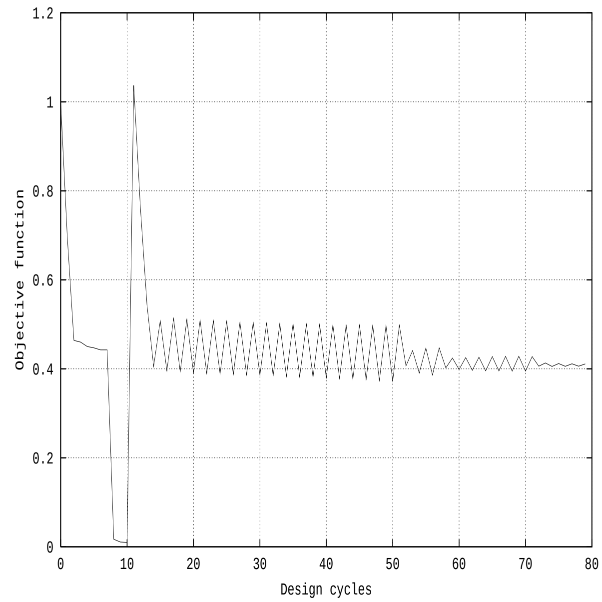

Figure 6: Objective function evolution

subject to a minimum thickness constraint. Hence, the objective function was defined as:

$$\begin{aligned} &\text{Minimize } L = w_1 \frac{C_d}{C_d^*} + w_2 \frac{(C_l - C_l^*)^2}{C_l^{*2}} \\ &\text{Subject to } \; t(\boldsymbol{x}) \leq f(x)\; g(z) \quad , \end{aligned} \tag{44}$$

where w_1 and w_2 are the weights given to the drag and to the lift parts of L, respectively. C_d^* is the initial drag force and C_l^* its lift counterpart. The inital wing geometry and mesh are presented in 4. The minimum thickness is defined by the functions $f(x)$ and $g(z)$. The first one is a quadratic function in the x direction, which reachs its maximum value at the middle edge of the wing (vertical plane that passes through the points $(0.5, 0, 0)$ and $(0.95, 0, 0.9)$), and with a value of zero at the leading and trailing edges. The second function ($g(z)$), is linear in the z coordinate, with a value of one at the plane $z = 0$, and a value of zero at $z = 0.9$. Other enforced geometric constraints were imposed: Points at $(0, 0, 0)$ and $(1, 0, 0)$ (leading and trailing edge points on $z = 0$) remain fixed, points at $z = 0$ can move only on this plane, and points at the leading and trailing edge allow to move only in the vertical direction (y direction). The rest of the points are also only allowed to move in the normal direction to $\mathcal{S}$.

Figure 5 shows the initial and final wing geometries after 80 design cycles (the number of design parameters where approximately 3575). The design was mostly dominated by the minimum thickness contraint, even though some small twist and asymmetry were also obtained. The objective function gradients were computed using an incomplete continuous adjoint formulation. The final of the design process were considered when the drag and the lift forces did not present more meaningful variations. The drag improvement was of a 60%, which was obtained with a 9% of lift increment. Figure 6 shows the objective function evolution. It can be noticed that at the beginning of the design process the objective function value quickly decreased. This was due to the fact that the drag force decreased very fast, but in the same manner, the lift coeficient increased to a 14% (w_1 and w_2 were both set to 1). Hence, the weights (see (44)) were adjusted to $w_1 = 10^{-8}$ and $w_2 = 1$, and 3 design cycles were done (cycles 9 to 11) to adjust the lift at an admisible value. The weights were both set to one again, and an oscilatory behaviour was obtained mainly due to the fact that the parameter of the steepest descendent algorithm was kept constant (cycles 12 to 51). Therefore, such a parameter was reduced (twice) until a converged solution was obtained.

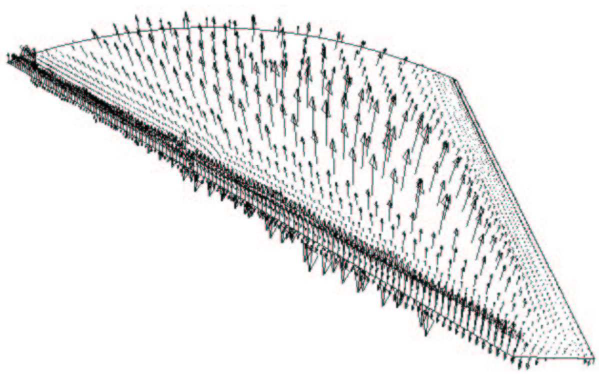

Figure 7: Non-smoothed objective function gradients at the initial geometry

Figures 7 and 8 illustrate how the improved pseudo-shell approach smooths the gradients to obtain wave-free surfaces. The "physical" properties used in this example were $\mu = 1$ and $\gamma = 0.3$ (see (40)), which can be considered as the standard ones. In most of the design cycles, the minimum thickness constraint had to be enforced by using Algorithm 1.

7 Conclusions

Some general continuous expressions to obtain the gradient of any given objective function with respect to some set of design parameters were deduced. The expressions

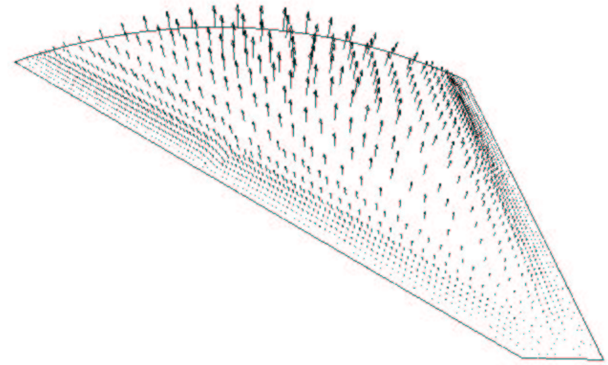

Figure 8: Smoothed objective function gradients (using the improved pseudo-shell approach) at the initial geometry

only use the values of the adjoint and flow fields at the objective surface (surface where the objective function is defined). Moreover, the error that one incurs when using different types of incomplete gradients was well defined.

An improved pseudo-shell approach to move the objective surface, and to impose general geometric constraints was shown. By construction, such an approach produces smooth shapes in each design cycle.

Two numerical examples were presented to demonstrate the methodology developed.

References

[1] W. Anderson and D. Bonhaus. Airfoil design on unstructured grids for turbulent flows. *NASA TM 112867*, 1997.

[2] W. Anderson and V. Venkatakrishnan. Aerodynamic design optimization on unstructured grids with a continuous adjoint formulation. *ICASE report No. 97-9*, 1997.

[3] J. Elliot and J. Peraire. Practical three-dimensional aerodynamic design and optimization using unstructured meshes. *AIAA journal*, 35:1479–1485, 1997.

[4] R. Glowinski and O. Pironneau. On the numerical computation of the minimum-drag profile in laminar flow. *J. Fluid Mech.*, 72:385–389, 1975.

[5] A. Jameson. Optimum aerodynamic design using CFD and control theory. *AIAA-95-1729-CP*, 1995.

[6] A. Jameson and S. Kim. Reduction of the adjoint gradient formula in the continuous limit. *AIAA-2003-0040*, 2003.

[7] G. Kuruvila, S. Ta'asan, and M. Salas. Airfoil design and optimization by the one-shot method. *AIAA-95-0478*, 1995.

[8] R. Löhner, O. Soto, and C. Yang. An adjoint-based design methodology for cfd optimization problems. *AIAA-03-0299*, 2003.

[9] T. Matsuzawa and H. Hafez. Treatment of shock waves in design optimization via adjoint equation approach. *AIAA-98-2537*, 1998.

[10] B. Mohammadi. Dynamical approaches and incomplete gradients for shape optimization and flow control. *AIAA-99-3374*, 1999.

[11] B. Mohammadi and O. Pironneau. *Applied Shape Optimization for Fluids.* Oxford Sciences publications, 2001.

[12] S. Nadarajah and A. Jameson. Studies of the continuous and discrete adjoint approaches to viscous automatic aerodynamic shape optimization. *AIAA-2001-2530*, 2001.

[13] R. Narducci, B. Grossman, M. Valorani, A. Dadone, and R. Haftka. Optimization methods for non-smooth or noisy objective functions in fluid design problems. *AIAA-95-1648-CP*, 1995.

[14] E. Nielsen. *Aerodynamic design sensitivities on an unstructured mesh using the Navier-Stokes equations and a discrete adjoint formulation.* PhD thesis, Virginia Polytechnic Institute and State University, 1998.

[15] E. Nielsen and W. Anderson. Aerodynamic design optimization on unstructured meshes using the Navier-Stokes equations. *AIAA-98-4809*, 1998.

[16] O. Pironneau. On optimum profiles in Stokes flow. *J. Fluid Mech.*, 59:117–128, 1973.

[17] O. Pironneau. On optimum profiles in Fluid Mechanics. *J. Fluid Mech.*, 64:97–110, 1974.

[18] J. Reuter, J. Alonso, J. Martins, and S. Smith. A couple aero-structural optimization method for complete aircraft configurations. *AIAA-99-0187*, 1999.

[19] J. Reuter, A. Jameson, J. Alonso, M. Rimlinger, and D. Saunders. Constrained multipoint aerodynamic shape optimization using and adjoint formulation and parallel computers. *AIAA-97-0103*, 1997.

[20] J. Reuter, A. Jameson, J. Farmer, L. Martinelli, and D. Saunders. Aerodynamic shape optimization of complex aircraft configurations via an adjoint formulation. *AIAA-96-0094*, 1996.

[21] M. Rizk. CFD optimization by sensitivity derivatives evaluated from finite-difference jacobians. *AIAA-95-1691-CP*, 1995.

[22] O. Soto and R. Löhner. CFD optimization using an incomplete-gradient adjoint approach. *AIAA-00-0666*, 2000.

[23] O. Soto and R. Löhner. CFD shape optimization using an incomplete-gradient adjoint formulation. *Int. J. Numer. Meth. Engrg.*, 51:735–753, 2001.

[24] O. Soto and R. Löhner. General methodologies for incompressible flow design problems. *AIAA-2001-1061*, 2001.

[25] O. Soto and R. Löhner. A mixed adjoint formulation for incompressible turbulent problems. *AIAA-02-0451*, 2002.

[26] O. Soto, R. Löhner, and C. Yang. A stabilized pseudo-shell approach for surface parametrization in cfd design problems. *Comm. in Numer. meth. in Eng.*, 18:Issue 4, 2002.

[27] O. Soto, R. Löhner, and C. Yang. An adjoint-based design methodology for cfd problems. *Int. J. of Num. Meth. for Heat and Fluid Flow*, Accepted for publication, 2003.