Arthur Shiniti Cato

**Adjoint method to compute non-geometric
sensitivities in time-dependent compressible flows**

São Paulo
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Fluid Mechanics

Supervisor:

Prof. Dr. Ernani Vitillo Volpe

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I dedicate this work to my wife, my
parents and my sisters.

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RESUMO

O cálculo de sensibilidades é essencial para muitos dos métodos de otimização aerodinâmica. Em particular, ter conhecimento sobre as derivadas de funções de mérito (usualmente ligadas a sustentação, arrasto, distribuição de pressão etc.) com respeito às condições de contorno permite mapear regiões de operação ótima. O presente trabalho estuda o método adjunto em sua formulação contínua e sua aplicação em escoamentos compressíveis tempo-dependentes, permitindo o cálculo de sensibilidades relacionadas aos parâmetros de controle impostos nas fronteiras permeáveis. Para tal, as equações adjuntas e suas condições de contorno são desenvolvidas com a finalidade de estabelecer um problema bem-posto, tomando-se proveito de sua formulação característica e resolvendo um problema de Riemann completo. Neste estudo, as equações são resolvidas discretizando o domínio espacial com o método de volumes finitos, enquanto que a integração temporal é feita com base em um esquema Runge-Kutta de 5 passos e segunda ordem de precisão. Calcula-se, finalmente, o gradiente das funções de mérito com respeito aos parâmetros impostos nas fronteiras para alguns exemplos de aplicação.

Palavras chave: Método adjunto, escoamento compressível, aerodinâmica, dinâmica dos fluidos computacional, sensibilidades.

ABSTRACT

Sensitivity gradients are essential for many of the aerodynamic optimization methods. In particular, the information about the derivatives of functionals (usually related to the lift, drag, pressure distribution etc.) with respect to the boundary conditions allows one to determine regions of optimal operation. The present work studies the adjoint method in its continuous formulation and its application to time-dependent compressible flows; the method is used to compute sensitivities related to the control parameters imposed on the permeable boundaries. The adjoint equations and their boundary conditions are developed to establish a well-posed problem. It is used the characteristic formulation and the complete Riemann problem. The equations are solved by discretizing the spatial domain a finite volume method and the temporal integration is based on a 5-step Runge-Kutta scheme and second order of precision. Finally, the gradient of the function of merit is computed with respect to the parameters imposed at the boundaries for some examples.

Keywords: Adjoint method, compressible flow, aerodynamics, computational fluid dynamics, sensitivities.

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1 INTRODUCTION

The sensitivity analysis is essential to optimization design problems and study of systems stability, being an extensive field of research by itself. In what concerns the sensitivity analysis in aerodynamics, one of the many techniques used to compute gradients is the so called adjoint method, which development in the field was firstly driven by the shape optimization problem of aerodynamic surfaces. The objective of this chapter is to expose the aerodynamic optimization scenario, placing in context the importance and difficulties of computing sensitivities. The adjoint method used to calculate such derivatives and its formulation in two different ways (the traditional development by Jameson (1988) [1] and the generalized formalization made by Cacuci (1980) [2] are presented and discussed.

1.1 Aerodynamic optimization

An aerodynamic design method, whether analytical, numerical or experimental, consists in a performance optimization. Despite the existent particularities in each case, the measure of performance usually adopted resides in a cost functional, also called a measure of merit or objective functional (Reuther, 1996) [3]. The improvement of such functional must be so as the set of constraints in the problem are satisfied.

The first methods in which the study of flight aerodynamics has been based were the experimental ones. However, the growth of mathematical and numerical tools concerning the studies of fluid flows, notably the Computational Fluid Dynamics or CFD, made possible a substantial progress in the development of aerodynamic surfaces (Reuther, 1996) [3]. With both simulations and empirical data, the robustness of airfoils, wings and turbo-machinery increased rapidly.

Although accurate solutions to highly non-linear flow regimes can be found with the help of CFD, its application in the direct aerodynamic shape optimization is still limited (Reuther, 1996) [3].

While the numerical tools become more robust, the problems engineers have to deal with also increases in complexity. One of the major difficulties is the computational cost management. Hence, the study of different numerical techniques is a main domain of research. The engineers must, then, find the appropriate methods (in terms of advantage and disadvantages) given a certain problem and practical constraints (such as computational capacity, time, accuracy etc.).

As a problem under investigation, the techniques in aerodynamics optimization are constantly being sophisticated. Steady flows regime is a common place to most of the developments in these techniques, either by the natural way as it appears in the mathematical and physical models used in a variety of cases or by the simplification to deal with the complexity of a specific problem (in general both happen together). However, there are cases in which unsteadiness can't be neglected or, actually, is the focus of the problem, as it can be seen in helicopter rotors and turbo-machinery blades (Nadarajah and Jameson, 2007) [4].

These types of machines work with unsteady flows and loads. Shape optimization is interesting to decrease the effects of fluttering, buffeting, poor gust, acoustic response or dynamic stall (Nadarajah and Jameson, 2007) [4].

In Reuther (1996) [3] some of the most usual methods in aerodynamic optimization are highlighted and characterized. Two of them are: Inverse Methods and Numerical Optimization Methods.

1.1.1 Inverse Methods

Before the current computational tools were available, the usual strategy to optimize an aerodynamic shape was to use a base geometry which would be tested in wind tunnels. After the studies of the data acquired, the geometry would undergo changes until it could achieve a satisfactory performance under the imposed constraints.

The inverse methods trace an opposite path. Under the imposed constraints and aiming a certain achievement, its calculated the shape which will better gives the desired result. Briefly, these inverse methods can be classified as inverse surface methods or inverse field methods. The first one searches a shape that gives a specified distribution of an aerodynamic quantity over a surface (e.g. pressure) while the second one relies in an objective or constraint that is imposed on the whole flow-field.

1.1.2 Numerical Optimization Methods

Numerical optimization approaches can be categorized into heuristic and gradient-based methods (Walther and Nadarajah, 2012) [5]. The heuristic methods are focused only on the evaluation of the cost-functional. They usually require a large amount of computational cost due to the numerous evaluations needed to an optimum converged solution. The gradient-based methods are based from the derivatives of the cost-functional with respect to the design variables, being able to find a local optimum with usually fewer iterations. However, if there is a large number of these design variables one can have difficulties to compute the gradient.

The gradient-based methods consist in the use of an optimization technique working together with a CFD code in such a way as to constantly modify a set of design variables until it maximizes a design objective.

One way to obtain approximated values for the gradient components is by finite differences. One can impose a perturbation in each one of the design variables separately and calculate the corresponding change in the objective function with a CFD algorithm. The gradient gives the information of what direction one must follow to maximize (or minimize) the objective, that way some of the most common optimization techniques profit from that, such as steepest descent, conjugate gradient or quasi-Newton. Notice that the CFD flow analysis must run repeatedly until the norm of the gradient shows convergence to zero (or the improvement becomes impossible).

As this class of methods allows a relative versatility concerning the chosen measure of merit (Reuther, 1996) [3], it can be used in place of inverse methods once one can define the functional to be minimize as the difference between a target and an actual aerodynamic property distribution or maximize a field-flow based functional.

1.2 Sensitivity Theory in Aerodynamics

The shape optimization problem presented in the previous section was one of the pillars that motivated the numerical sensitivity analysis in aerodynamics or, in other words, the evaluation of derivatives of output quantities (Peters and Wight, 2010) [6]. These quantities are usually defined by surface integrals (lift, drag etc.).

The sensitivity analysis, however, can be extended to control parameters which are not related to a shape function of a aerodynamic geometry. Common examples are the

stability derivatives, which give information about how much a quantity (as a force or momentum) can be modified by a change in flight conditions (e.g. the angle of attack, altitude, pressure, speed etc.).

Methods to compute numerical sensitivities in CFD codes can be also used to refine grids efficiently (Ringue and Nadarajah, 2018) [7], estimating the sensitivity of the error between the actual and numerical solution in relation to the type and size of the grid elements or the polynomial degree distributions.

Some of the fundamental methods with the purpose of computing sensitivities are presented: the finite differences method, which can be considered the simplest one regarding the numerical formulation; the adjoint method formulated for optimal design problems, firstly developed with the purpose to compute optimal geometries in aerodynamics; and the adjoint method extended to general systems (when general boundary conditions are considered control parameters besides just the geometric ones). Evidently, the general formulation of the adjoint method includes the particular one, nevertheless they are presented separately due to the distinct approaches usually seen in the literature.

1.2.1 Finite Differences

The finite differences method is the simplest way to compute gradients, since it does not require any modification of the solver. On considering a set of control parameters P_i , one has to solve the flow for the corresponding perturbations $P_i + \delta P_i$ and $P_i - \delta P_i$ considered separately. If the cost functional is represented by I , the sensitivity $\frac{dI}{dP_i}$ can be simply approximate by finite differences. For instance, one approximation can be:

$$\frac{dI}{dP_i} \approx \frac{[I(P_i + \delta P_i) - I(P_i - \delta P_i)]}{2\delta P_i} \quad (1.1)$$

It is evident that for an expressive number of parameters P_i , the computational cost becomes impracticable.

1.2.2 Adjoint Method for Optimal Design Problems

The work on control theory applied to systems governed by partial differential equations advanced by Lions (1971) [8] introduced the theoretical basis to the adjoint methods. As the name suggests, it consists in solving an adjoint system of equations. Approaching design problems in the field of fluid dynamics with adjoint equations was first developed by

Pironneau (1984) [9] for elliptic systems. In aeronautical engineering, with the advances in CFD, the use of the method was extended by Jameson (1988) [1].

The adjoint method traditionally proposed in aerodynamics shape optimization is, in essence, a design problem identified as a control problem. In this context, the system is controlled by geometric parameters (e.g., coefficients from an aerofoil shape function) as presented by Jameson (1988) [1]. The particular way it is developed in this section implies that only geometric sensitivities pertinent to the aerodynamic shape surface can be calculated. To elucidate the latter affirmation, one can assume that the geometry of the aerodynamic surface is expressed as:

$$f(x) = \sum a_i b_i(x) \quad (1.2)$$

Where a_i are weights of shape functions $b_i(x)$. The cost functional I , which can be related, for example, to the drag force, depends on the a_i , even if not directly. In order to optimize the shape function, it is needed to compute the derivatives $\frac{dI}{da_i}$. The adjoint method proposed is, then, restrained to compute the sensitivities of this type of problem.

Now, consider a flow over an airfoil. The set of cost functions of interest are the ones associated with the aerodynamic properties, usually defined as surface integrals (e.g. drag force, lift force etc.). This implies that the objective I is a function of the flow-field variables, denoted as a vector $\mathbf{Q}$, and the geometry of the boundary, denoted as a function $\mathcal{F}$:

$$I = I(\mathbf{Q}, \mathcal{F}) \quad (1.3)$$

A variation of I is given by:

$$\delta I = \left[\frac{\partial I^T}{\partial \mathbf{Q}} \right]_I \delta \mathbf{Q} + \left[\frac{\partial I^T}{\partial \mathcal{F}} \right]_{II} \delta \mathcal{F} \quad (1.4)$$

As developed by Jameson (2003) [10], it's interesting to indicate the portion of the total variation due to the variation of the flow-field solution, subscript I , and the one due to the shape change, subscript II . The second one is easier to derive, since the cost function can usually be expressed directly in terms of the shape function, this is not applicable to the first term.

Assume the system is governed by a set of partial differential equations (PDEs), which

can be cast in operator form as:

$$R(\mathbf{Q}, \mathcal{F}) = 0 \quad (1.5)$$

The first variation of R is given in an analogous form as equation 1.4.

$$\delta R = \left[\frac{\partial R}{\partial \mathbf{Q}} \right]_I \delta \mathbf{Q} + \left[\frac{\partial R}{\partial \mathcal{F}} \right]_{II} \delta \mathcal{F} = 0 \quad (1.6)$$

The use of a Lagrange multiplier vector applied to the governing equations operator as a form of constraint to the cost function implies:

$$\begin{aligned} \delta I &= \frac{\partial I^T}{\partial \mathbf{Q}} \delta \mathbf{Q} + \frac{\partial I^T}{\partial \mathcal{F}} \delta \mathcal{F} - \Psi^T \left(\frac{\partial R}{\partial \mathbf{Q}} \delta \mathbf{Q} + \frac{\partial R}{\partial \mathcal{F}} \delta \mathcal{F} \right) \Leftrightarrow \\ \delta I &= \left(\frac{\partial I^T}{\partial \mathbf{Q}} - \Psi^T \frac{\partial R}{\partial \mathbf{Q}} \right)_I \delta \mathbf{Q} + \left(\frac{\partial I^T}{\partial \mathcal{F}} - \Psi^T \frac{\partial R}{\partial \mathcal{F}} \right)_{II} \delta \mathcal{F} \end{aligned} \quad (1.7)$$

Clearly the addition of δR doesn't change the variation of the cost function since $\delta R = 0$. Nevertheless, the variation of the flow-variables, $\delta \mathbf{Q}$, must be admissible or realisable. Equation (1.7) is rearranged by separating the flow-field variations from the geometric ones.

Ψ is chosen so as to satisfy the adjoint equation:

$$\left[\frac{\partial R}{\partial \mathbf{Q}} \right]^T \Psi = \frac{\partial I}{\partial \mathbf{Q}} \quad (1.8)$$

One obtains the variation of the objective function written as:

$$\delta I = \mathcal{G} \delta \mathcal{F} \quad (1.9)$$

Where

$$\mathcal{G} = \left(\frac{\partial I^T}{\partial \mathcal{F}} - \Psi^T \frac{\partial R}{\partial \mathcal{F}} \right) \quad (1.10)$$

That being presented, one has a description of a method to compute sensitivities of the objective functional. Before proceeding to the time-dependent case, some notes are important to be highlighted. As described by Jameson (2003) [10]:

1. Equation (1.9) is independent of $\delta \mathbf{Q}$. Consequently, the gradient of I with respect to an arbitrary number of design variables can be computed without the necessity of additional flow-field evaluation.
2. If the governing equations are differential partial equations, then the adjoint equations are also partial differential and the boundary conditions have to be carefully treated.

In order to extend the analysis to a time-dependent problem, one can consider that the cost function can be written as:

$$I = \frac{1}{T} \int_0^{t_f} \mathcal{L}(\mathbf{Q}, \mathcal{F}) dt + \mathcal{M}[\mathbf{Q}(t_f)] \quad (1.11)$$

The functional defined is a sum of time-average functions represented by $\mathcal{L}(\mathbf{Q}, \mathcal{F})$, while $\mathcal{M}[\mathbf{Q}(t_f)]$ is a function of the solution $\mathbf{Q}(t)$ at $t = t_f$, the final time (Nadarajah and Jameson, 2007) [4].

When the shape function $\mathcal{F}$ is changed, the cost function varies by:

$$\delta I = \frac{1}{T} \int_0^{t_f} \left(\frac{\partial \mathcal{L}^T}{\partial \mathbf{Q}} \delta \mathbf{Q} + \frac{\partial \mathcal{L}^T}{\partial \mathcal{F}} \delta \mathcal{F} \right) dt + \frac{\partial \mathcal{M}^T}{\partial \mathbf{Q}} \delta \mathbf{Q}(t_f) \quad (1.12)$$

Consider that the governing equations are now time-dependent as well:

$$V \frac{\partial}{\partial t} \mathbf{Q} + R(\mathbf{Q}, \mathcal{F}) = 0 \quad \text{with } V \text{ some constant} \quad (1.13)$$

Its first variation is:

$$\delta R = V \frac{\partial}{\partial t} \delta \mathbf{Q} + \left[\frac{\partial R}{\partial \mathbf{Q}} \right] \delta \mathbf{Q} + \left[\frac{\partial R}{\partial \mathcal{F}} \right] \delta \mathcal{F} = 0 \quad (1.14)$$

Notice that equations (1.4) and (1.6) are the special cases of equations (1.12) and (1.14) when one is dealing with a steady-state flow.

If a Lagrange multiplier is applied at equation (1.14) and integrated in time, it follows that:

$$\frac{1}{T} \int_0^{t_f} \Psi^T \left(V \frac{\partial}{\partial t} \delta \mathbf{Q} + \left[\frac{\partial R}{\partial \mathbf{Q}} \right] \delta \mathbf{Q} + \left[\frac{\partial R}{\partial \mathcal{F}} \right] \delta \mathcal{F} \right) dt = 0 \quad (1.15)$$

And the first variation of the objective functional constrained by the governing equations becomes:

$$\begin{aligned} \delta I = & \frac{1}{T} \int_0^{t_f} \left(\frac{\partial \mathcal{L}^T}{\partial \mathbf{Q}} \delta \mathbf{Q} + \frac{\partial \mathcal{L}^T}{\partial \mathcal{F}} \delta \mathcal{F} \right) dt + \frac{\partial \mathcal{M}^T}{\partial \mathbf{Q}} \delta \mathbf{Q}(t_f) + \\ & - \frac{1}{T} \int_0^{t_f} \Psi^T \left(V \frac{\partial}{\partial t} \delta \mathbf{Q} + \left[\frac{\partial R}{\partial \mathbf{Q}} \right] \delta \mathbf{Q} + \left[\frac{\partial R}{\partial \mathcal{F}} \right] \delta \mathcal{F} \right) dt \end{aligned} \quad (1.16)$$

In order to make the gradient expression free from reevaluation of the flow-field variables, the term given by

$$\frac{1}{T} \int_0^{t_f} \Psi^T V \frac{\partial}{\partial t} \delta \mathbf{Q} dt \quad (1.17)$$

is integrated by parts. The result is:

$$\begin{aligned} \delta I = & \frac{1}{T} \int_0^{t_f} \left(\frac{\partial \mathcal{L}^T}{\partial \mathbf{Q}} + V \frac{\partial \Psi^T}{\partial t} - \Psi^T \left[\frac{\partial R}{\partial \mathbf{Q}} \right] \right) \delta \mathbf{Q} dt + \\ & + \left(\frac{\partial \mathcal{M}^T}{\partial \mathbf{Q}} + \frac{V}{T} \Psi^T(t_f) \right) \delta \mathbf{Q}(t_f) + \frac{1}{T} \int_0^{t_f} \left(\frac{\partial \mathcal{L}^T}{\partial \mathcal{F}} - \Psi^T \left[\frac{\partial R}{\partial \mathcal{F}} \right] \right) \delta \mathcal{F} dt \end{aligned} \quad (1.18)$$

Finally, the adjoint equation is given by:

$$V \frac{\partial \Psi}{\partial t} - \left[\frac{\partial R}{\partial \mathbf{Q}} \right] \Psi = - \frac{\partial \mathcal{L}}{\partial \mathbf{Q}} \quad (1.19)$$

With the terminal condition as:

$$\frac{V}{T} \Psi(t_f) = - \frac{\partial \mathcal{M}}{\partial \mathbf{Q}} \quad (1.20)$$

And one can write:

$$\delta I = \mathcal{G}^T \delta \mathcal{F} \quad (1.21)$$

Where

$$\mathcal{G}^T = \frac{1}{T} \int_0^{t_f} \left(\frac{\partial \mathcal{L}^T}{\partial \mathcal{F}} - \Psi^T \frac{\partial R}{\partial \mathcal{F}} \right) dt \quad (1.22)$$

The equation (1.10) is the steady case of (1.22). A key point in optimal control of

time-dependent problems is that one needs to solve an adjoint equation in a reverse time with reference of the physical solution, considering the terminal boundary condition given by the latter.

1.2.3 Adjoint Method for General Systems

If one wants to compute derivatives with respect to more general parameters besides the geometric ones described in the previous section, it is necessary to generalize the adjoint method. The present development was made by Cacuci (1980) [2] and it takes account the boundary conditions as control parameters. This adjustment allows the calculation of sensitivities with respect to parameters at the permeable boundaries. The work of Cacuci (1980) [2] formalizes the theory behind the adjoint method proposed by Jameson (1988) [1].

Assume a general problem as described by a set of n non-linear PDE's and subject by a set of boundary conditions. It can be represented symbolically as:

$$\begin{aligned} \mathbf{N}[\mathbf{Q}(\chi, t), \mathbf{P}] &= \mathbf{R}(\chi, \mathbf{P}) \\ \mathbf{B}[\mathbf{Q}(\chi, t), \mathbf{P}]_s &= 0 \end{aligned} \quad (1.23)$$

Where the $\mathbf{Q}$ vector represents the coordinates of the system in the state-space, whereas χ represents the coordinates in the phase-space. The vector $\mathbf{P}$ is composed by the control or input parameters.

$$\begin{aligned} \mathbf{Q}(\chi) &= [Q_1(\chi), \dots, Q_n(\chi)] \\ \mathbf{P}(\chi) &= [P_1(\chi), \dots, P_m(\chi)] \\ \chi &= (\chi_1, \dots, \chi_i) \end{aligned} \quad (1.24)$$

One can notice that the set of equations $\mathbf{N}$ and $\mathbf{B}$ are both functions of the state variables and the control parameters. The hypotheses that the boundary conditions depend on the control parameters is the generalization needed to compute non-geometric sensitivities, differently from the traditional approach that is used in geometric optimization.

The measure of merit can be described as a functional of form:

$$I[\mathbf{Q}, \mathbf{P}] = \frac{1}{T} \int_{t_0}^{t_f} \int_{\chi} \mathcal{F}[\mathbf{Q}(\chi, t), \mathbf{P}(\chi, t), \chi] d\chi dt \quad (1.25)$$

Where $\mathcal{F}$ is function of the state variables and the control parameters. In aerodynamics this integral is normally associated to time average surface forces, quadratic errors between a target and actual distribution of pressure, kinetic energy etc. (as in the previous cases).

To proceed further, one shall assume that $\mathbf{Q}$ and $\mathbf{P}$ are elements of Hilbert spaces $H_1 = [L^2(I_i)]^n$ and $H_2 = [L^2(I_i)]^m$ (Cacuci et al., 1980) [2]. In this notation I_j is the domain of vector χ with dimension j and $[L^2(I)]^k$ represents the space of Lebesgue square integrable vector functions of dimension k defined in the domain I .

One can compute the first Gateaux variation:

$$\delta I = \frac{1}{T} \left[\int_{t_0}^{t_f} \int_{\chi} \mathcal{F}'_{\mathbf{Q}} \delta \mathbf{Q} d\chi dt + \int_{t_0}^{t_f} \int_{\chi} \mathcal{F}'_{\mathbf{P}} \delta \mathbf{P} d\chi dt \right] \quad (1.26)$$

The quantities $\mathcal{F}'_{\mathbf{Q}}$ and $\mathcal{F}'_{\mathbf{P}}$ represent vectors whose components are the Fréchet derivatives of $\mathcal{F}$ with respect to the corresponding Q_i and P_i . The first term of the right side is the direct variation of the measure of merit due to a variation of the state vector (physical part); in an analogous way, the second term is the direct variation due to a variation of the control parameters (parametric part). On denoting them as $\delta I_{\mathbf{Q}}$ and $\delta I_{\mathbf{P}}$, one gets, respectively:

$$\delta I = \delta I_{\mathbf{Q}} + \delta I_{\mathbf{P}} \quad (1.27)$$

The equation above is the same as equation (1.4). From now on, an inner product is defined in the whole domain Ω and on its boundaries $\partial\Omega$ as:

$$\begin{aligned} \langle \mathbf{F}, \mathbf{G} \rangle &= \int_{\Omega} \mathbf{F} \cdot \mathbf{G} d\Omega = \int_{t_0}^{t_f} \int_{\mathcal{V}} \mathbf{F} \cdot \mathbf{G} d\mathcal{V} dt \\ \langle \mathbf{F}, \mathbf{G} \rangle_S &= \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{G} d\Omega = \int_{t_0}^{t_f} \int_S \mathbf{F} \cdot \mathbf{G} dS dt \end{aligned} \quad (1.28)$$

The augmented functional is constructed by imposing the constraints, which yields:

$$G = I[\mathbf{Q}, \mathbf{P}] - \langle \Phi, \mathbf{N} - \mathbf{R} \rangle - \langle \Psi, \mathbf{B} \rangle_s - \langle \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle \quad (1.29)$$

The variables Φ , Ψ and $\mathbf{a}$ are Lagrange multipliers, which correspond to the constraints given by, respectively, the governing equations, the boundary conditions and the set of prescribed values of control parameters in a baseline configuration $\mathbf{P} - \mathbf{P}_0$.

To calculate the variation of equation (1.29) it is required to determine $\delta\mathbf{Q}$. Where the latter comes from the Fréchet derivatives of the flow governing equations and boundary conditions thereof, (1.23). Those derivatives lead to the expressions:

$$\begin{aligned}\mathbf{L}\delta\mathbf{Q} &= \mathbf{S}\delta\mathbf{P} \\ \mathbf{B}'_{\mathbf{Q}}\delta\mathbf{Q} &= -\mathbf{B}'_{\mathbf{P}}\delta\mathbf{P}\end{aligned}\tag{1.30}$$

Where the operators $\mathbf{L}$ and $\mathbf{S}$ can be represented as matrices whose components are:

$$\begin{aligned}L_{kr} &= (N_k)'_{Q_r} & k = 1, \dots, n; \quad r = 1, \dots, n \\ S_{kr} &= (Q_k)'_{P_r} - (N_k)'_{P_r} & k = 1, \dots, n; \quad r = 1, \dots, m\end{aligned}\tag{1.31}$$

The variation of equation (1.29) can be computed by taking the variation of each term. The variation of the constraint that refers to the governing equations is:

$$\delta\langle\Phi, \mathbf{N} - \mathbf{R}\rangle = \langle\delta\Phi, \mathbf{N} - \mathbf{R}\rangle + \langle\Phi, \mathbf{L}\delta\mathbf{Q}\rangle - \langle\Phi, \mathbf{S}\delta\mathbf{P}\rangle\tag{1.32}$$

An adjoint operator $\mathbf{L}^*$ of $\mathbf{L}$ can be defined as:

$$\langle\Phi, \mathbf{L}\delta\mathbf{Q}\rangle = \langle\mathbf{L}^*\Phi, \delta\mathbf{Q}\rangle - P[\Phi, \delta\mathbf{Q}]_s\tag{1.33}$$

Where $P[\Phi, \delta\mathbf{Q}]_s$ is called a bilinear concomitant calculated in the boundary. The advantage of using the adjoint operator is that one can write the variation of (1.29) in terms of the solution Φ from the adjoint problem.

The variation of the second and third terms of the RHS of equation (1.29) yields to the following expressions:

$$\delta\langle\Psi, \mathbf{B}\rangle_s = \langle\delta\Psi, \mathbf{B}\rangle_s + \langle\Psi, \mathbf{B}'_{\mathbf{Q}}\delta\mathbf{Q}\rangle_s + \langle\Psi, \mathbf{B}'_{\mathbf{P}}\delta\mathbf{P}\rangle_s\tag{1.34}$$

$$\delta\langle\mathbf{a}, \mathbf{P} - \mathbf{P}_0\rangle = \langle\delta\mathbf{a}, \mathbf{P} - \mathbf{P}_0\rangle + \langle\mathbf{a}, \delta\mathbf{P}\rangle\tag{1.35}$$

By introducing the inner product definition (1.28) into the equation (1.25) and taking the variation of (1.29), while substituting eqs. (1.32) - (1.35) for their counterparts, leads to the following:

$$\begin{aligned}
\delta G = & \langle \mathcal{F}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle + \langle \mathcal{F}'_{\mathbf{P}}, \delta \mathbf{P} \rangle - \langle \delta \Phi, \mathbf{N} - \mathbf{R} \rangle - \langle \mathbf{L}^* \Phi, \delta \mathbf{Q} \rangle + \\
& + P [\Phi, \delta \mathbf{Q}]_s + \langle \Phi, \mathbf{S} \delta \mathbf{P} \rangle - \langle \delta \Psi, \mathbf{B} \rangle_s - \langle \Psi, \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_s + \\
& - \langle \Psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s - \langle \delta \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle - \langle \mathbf{a}, \delta \mathbf{P} \rangle
\end{aligned} \tag{1.36}$$

The bilinear concomitant defined in equation (1.33) arises from the integration by parts currently used to find the adjoint operator. As one would be interested in eliminating the term related to the variation of state variables on the boundaries, a convenient decomposition proposed by Cacuci *et al.* (1980) [2] is given by:

$$P [\Phi, \delta \mathbf{Q}]_s = \langle P_1 (\Phi), \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_s + \langle \mathbf{B}^* (\Phi), \mathbf{M} \delta \mathbf{Q} \rangle_s \tag{1.37}$$

The first term of the RHS of equation (1.37) indicates an inner product between an operator P_1 and the linearized physical boundary conditions operator. The second term is an inner product between the adjoint boundary conditions operator and $\mathbf{M} \delta \mathbf{Q}$, where $\mathbf{M}$ must be linearly independent from $\mathbf{B}'_{\mathbf{Q}}$.

Notice that the decomposition of the bilinear concomitant is not unique, as well as P_1 and $\mathbf{M}$. Substituting in (1.36) and rearranging:

$$\begin{aligned}
\delta G = & - \langle \delta \Phi, \mathbf{N} - \mathbf{R} \rangle - \langle \delta \Psi, \mathbf{B} \rangle_s - \langle \delta \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle - \langle \mathbf{L}^* \Phi - \mathcal{F}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle + \\
& - \langle \Psi, \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_s - [\langle P_1 (\Phi), \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_s + \langle \mathbf{B}^* (\Phi), \mathbf{M} \delta \mathbf{Q} \rangle_s] + \langle \Phi, \mathbf{S} \delta \mathbf{P} \rangle + \\
& \langle \mathcal{F}'_{\mathbf{P}}, \delta \mathbf{P} \rangle - \langle \Psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s - \langle \mathbf{a}, \delta \mathbf{P} \rangle
\end{aligned} \tag{1.38}$$

As described by Hayashi *et al.* (2016) [11], the extremes of the augmented functional are so that:

$$\delta G = 0 \quad \forall \quad \{\delta \mathbf{Q}, \delta \mathbf{P}, \delta \Phi, \delta \Psi, \delta \mathbf{a}\} \in \{\text{locus of realizability}\} \tag{1.39}$$

The implications to be satisfied are:

1. The vector $\mathbf{Q}$ satisfies the governing equations with boundary conditions (1.23) and the parameter vector is so that $\mathbf{P} = \mathbf{P}_0$, in other words, corresponding to the baseline configuration. The three first terms of the RHS of equation (1.38) are nulls.
2. On assuming

$$\Psi = -P_1 (\Phi) \tag{1.40}$$

The fifth and sixth terms cancel each other and Ψ can be solved in terms of Φ .

3. The adjoint equation and the adjoint boundary conditions must be satisfied by vector Φ . They are defined as:

$$\begin{aligned} \mathbf{L}^* \Phi - \mathcal{F}'_{\mathbf{Q}} &= 0 \\ \mathbf{B}^* (\Phi) &= 0 \end{aligned} \tag{1.41}$$

4. The vector $\mathbf{a}$ satisfies:

$$\langle \mathbf{a}, \delta \mathbf{P} \rangle = \langle \Phi, \mathbf{S} \delta \mathbf{P} \rangle + \langle \mathcal{F}'_{\mathbf{P}}, \delta \mathbf{P} \rangle - \langle \Psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s \tag{1.42}$$

which gathers the remaining variations when $\delta G = 0$.

Finally, as proved by Cacuci (1980) [2], $\langle \mathbf{a}, \delta \mathbf{P} \rangle$ is indeed the sensitivity function δI , meaning $\langle \mathbf{a}, \delta \mathbf{P} \rangle = \delta I$.

1.2.4 Continuous and Discrete Adjoint Method

The study of adjoint equations are based in two different formulations: continuous and discrete.

The continuous formulation takes place when the control theory is applied directly to the governing equations of the system. The adjoint equations are then discretized and solved. With the solution of the adjoint equation it is possible to get the necessary gradient information to proceed with the optimization algorithm.

On the other hand, the discrete adjoint equations can be obtained directly from the discretized flow governing equations.

Although it may be argued that the continuous formulation takes advantage of a procedure that is more intuitive to us, it seems that most of the literature on applications would rather favor the discrete approach. Quite different from the former, where one has to derive the adjoint pdes and boundary conditions thereof, the discrete approach boils down to a series of Matrix Transposition operations. These do not require integration by parts and, hence, it apparently does away with the need for adjoint boundary conditions and corresponding well-posedness considerations. As a matter of fact, the discrete adjoint can be (and it usually is) generated automatically and that is why it is the method of choice for multi-physics problems, where it could be exceedingly difficult to couple distinct sets of physics governing pdes. More detailed comparisons between the two formulations

are discussed in the work of Nadarajah and Jameson (2001 [12] and 1999 [13]).

The differences between them shall disappear when the mesh grid and time step approximate to zero.

1.3 Applications of the Adjoint Method

The main goals of the adjoint method were discussed as well as its theoretical formulation. To complement the literature review of the method, some of its practical applications are illustrated in several works as it shall be exposed in this section.

The first applications of both continuous and discrete adjoint method in aerodynamic optimization were developed for potential flows, Euler and Navier-Stokes equations in the works of Jameson (1988) [1], Reuther and Jameson (1994) [14], Jameson (1995) [15], Reuther and Jameson (1995) [16], Jameson, Pierce and Martinelli (1997) [17]. It is also worth mentioning the advantages of the adjoint method in unstructured grids in Jameson, Sriram and Martinelli (2003) [18].

Concerning the mathematical properties related to the adjoint equation, Giles and Pierce (1998 [19] and 2001 [20]) showed some considerations about the boundary conditions and the solution behaviour for the Euler adjoint equations (and the analytical solution for the Euler quasi-1D case).

As exemplified in the previous section about sensitivity theory in aerodynamics, the adjoint method became an interesting tool in error analyses. This field of study was first motivated by works such as Giles and Pierce (1998) [21], Giles and Pierce (1999) [22] and Giles and Süli (2002) [23]. The error analyses with the adjoint method showed to be useful in mesh refinement process (Venditti and Darmofal, 1999 [24]; Venditti and Darmofal, 2000 [25]; Venditti and Darmofal, 2001 [26]; Venditti and Darmofal, 2003 [27]; Ringue and Nadarajah, 2018 [7]).

Applications in unsteady flows are developed by Nadarajah and Jameson (2007) [4] and Kavvadias *et al.* (2015) [28]. For turbulent flows in unstructured grids, an important example is Martins, Alonso and Reuther (2005) [29].

1.4 About the Present Research

The present research has the objective of studying the adjoint method in order to compute sensitivities related to the flow properties at the permeable boundary conditions.

The works of Volpe and Santos (2009) [30] and Hayashi, Ceze and Volpe (2013) [31] established a procedure based on the characteristics of hyperbolic partial differential equations sets to derive the boundary conditions for the Euler adjoint equations. The purpose of the procedure was to conceive a well-posed adjoint problem, in the sense of Hadamard (1952) [32], according to the physical one.

On making use of the control theory for general systems developed by Cacuci *et al.* (1980) [2] and by pursuing the forgoing approach to ensure well-posedness, Hayashi (2016) [33] and Hayashi, Lima, Chierigatti and Volpe (2016) [11] proposed an alternative use of the adjoint method to compute general sensitivities in steady-state flows governed by the Euler Equations.

This research continues that series of studies, extending the idea from Hayashi (2016) [33] to unsteady flows, in which the boundary conditions are time-dependent. Thus, the present document overviews and reconstructs some of the ideas developed from the works cited above, while adding the time dependency condition.

Concerning the structure of the dissertation, the Chapter 2 is addressed to the theoretical aspects of the mathematical model used for the flow, in other words, the Euler's Equations. These equations are presented in its several formulations, including in generalized coordinates and in the characteristic form, the latter one being a key feature to the appropriate treatment of the boundary conditions. Chapter 3 presents the numerical method used to solve the Euler's Equations. In Chapter 4, the adjoint problem is obtained, using the method from Cacuci *et al.* (1980) [2] and Hayashi (2016) [33], but considering the time as playing an important role. Besides, a generalized formulation including control parameters at the outlet permeable boundaries is also presented. In Chapter 5, the numerical method to solve the adjoint problem is shown. The Chapter 6 is dedicated to the results obtained with the application of the method and, finally, Chapter 7 concludes the present study.

2 MATHEMATICAL MODEL OF THE FLOW

Although the full Navier-Stokes set usually represents the most complete model of flow physics, it may not be suitable for all problems of interest. This can be owed to unusual thermodynamic conditions or to computational cost limitations. In particular for unsteady aerodynamic flows that are largely driven by pressure, the Euler equations provide a very useful alternative. On the one hand, they neglect the dissipative mechanisms of viscosity and heat conductivity, thereby allowing significant reductions in computational costs. On the other, they capture the physics of advection and thermodynamics, but for dissipation. As the viscous effects are negligible compared to the inertial terms in many aerodynamic applications with sufficient large Reynolds numbers, the use of the Euler equations is natural. Moreover they are hyperbolic in space-time domain, as opposed to being of mixed character, as the Navier-Stokes equations. This makes their boundary problem and well-posedness conditions well defined, as long as it is cast in terms of Riemann variables and equations thereof. This particular aspect of the Euler equations plays a central role in the derivations that follow.

2.1 Navier-Stokes Equations

The Navier-Stokes equations are the description of the basic laws of conservation and balance in continuum mechanics. In other words, mass conservation, momentum equation and energy conservation. In terms of integral balances these equations are:

$$\begin{aligned}
 \int_{\Omega} \frac{\partial}{\partial t} \rho d\Omega + \oint_S \rho \vec{v} \cdot d\vec{S} &= 0 \\
 \int_{\Omega} \frac{\partial}{\partial t} \rho \vec{v} d\Omega + \oint_S (\rho \vec{v} \otimes \vec{v} + p) d\vec{S} &= \oint_S \vec{\tau} \cdot d\vec{S} + \int_{\Omega} \rho \vec{f}_e d\Omega \\
 \int_{\Omega} \frac{\partial}{\partial t} \rho e d\Omega + \oint_S \rho H \vec{v} \cdot d\vec{S} &= \oint_S (\vec{\tau} \cdot \vec{v}) \cdot d\vec{S} + \oint_S k \frac{\partial T}{\partial n} dS + \int_{\Omega} (\rho \vec{f}_e \cdot \vec{v} + q_H) d\Omega
 \end{aligned} \tag{2.1}$$

Where ρ is the specif mass, $\vec{v}$ the velocity field, p the pressure, $\bar{\tau}$ a stress tensor, $\vec{f}_e$ the volume forces at the control volume, H the enthalpy, e the total energy, k the heat transfer constant, T the temperature and q_H a source term.

On the basis of Reynolds Transport Theorem, we consider the case of a domain where there are no discontinuities like shock waves. Because at those discontinuities (which are assumed to have zero measure: 2-D surfaces in a 3-D domain) it is only the weak solutions that hold true, and they do that in the sense of distributions. That is, we consider a control volume of infinitesimal thickness that encloses the shock wave to study it.

Now, going back to portions of the domain that have no discontinuities, we argue that the volumetric balances should hold for control volumes of any size. Hence it implies that the kernel of the volume integrals of the above first principles should vanish identically there. Therefore we get the infinitesimal forms.

When applying Gauss Theorem to the integral form of Navier-Stokes equations one can find the differential conservative form. As the control volume is arbitrary, the Navier-Stokes Equations are locally valid at any point in the domain:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) &= 0 \\ \frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \otimes \vec{v} + p \vec{I} - \bar{\tau}) &= \rho \vec{f}_e \\ \frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho H \vec{v} - \bar{\tau} \cdot \vec{v} - k \nabla T) &= \rho \vec{f}_e \cdot \vec{v} + q_H \end{aligned} \quad (2.2)$$

Or in the Einstein notation and assuming a Newtonian fluid:

$$\begin{aligned} \partial_0 \rho + \partial_i (\rho v_i) &= 0 \\ \partial_0 (\rho v_i) + \partial_j (\rho v_j v_i) &= \rho f_i - \partial_i p + \partial_j \left(2\mu \left(\partial_{(j} v_{i)} - \frac{1}{3} \partial_k v_k \delta_{ji} \right) \right) \\ \partial_0 \left(\rho \left(e + \frac{1}{2} v_j v_j \right) \right) + \partial_i \left(\rho v_i \left(e + \frac{1}{2} v_j v_j \right) \right) &= \rho v_i f_i - \partial_i (p v_i) + \partial_i (k \partial_i T) \\ &+ \partial_i \left(2\mu \left(\partial_{(i} v_{j)} - \frac{1}{3} \partial_k v_k \delta_{ij} \right) v_j \right) \end{aligned} \quad (2.3)$$

2.2 Euler's Equations

The hypothesis of inviscid flow and no thermal conductivity applied to the Navier-Stokes equations give rise to a first-order system of non-linear coupled equations, called Euler's Equations.

The Euler equations, as the Navier-Stokes equations can be written in several ways according to the set of dependent flow variables. This set can be composed of the conservative variables (density, momentum and total energy), since these quantities obey the conservation laws. Another natural choice is the set of primitive variables (density, velocity and pressure), which can be easier to measure. Clearly, both are equivalents and can be derived from one another. Analogous to the previous section, it's presented the conservative formulations.

2.2.1 Integral Conservative Formulation

The integral formulation of the Euler equations obtained from taking the conservative variables, satisfying the conservation laws of mass, momentum and total energy. They can be written as follows:

$$\begin{aligned}
 \frac{\partial}{\partial t} \int_{\Omega} \rho d\Omega + \oint_S \rho \vec{v} \cdot d\vec{S} &= 0 \\
 \frac{\partial}{\partial t} \int_{\Omega} \rho \vec{v} d\Omega + \oint_S (\rho \vec{v} \otimes \vec{v} + p) d\vec{S} &= \int_{\Omega} \rho \vec{f}_e d\Omega \\
 \frac{\partial}{\partial t} \int_{\Omega} \rho e d\Omega + \oint_S \rho H \vec{v} \cdot d\vec{S} &= \int_{\Omega} \rho \vec{f}_e \cdot \vec{v} d\Omega
 \end{aligned} \tag{2.4}$$

The equations in the set are obtained neglecting the viscous terms in the Navier-Stokes equations and assuming no heat transfer or source term in the energy conservation.

To complete the system of equations presented, a constitutive relation is needed. The most common is the hypotheses of a gas that is thermally and calorically perfect, that is, an ideal gas that satisfies $p = \rho RT$ and has constant specific heats at constant pressure and volume. The ideal gas equations can also be cast in the form:

$$p = \left[e - \frac{1}{2} (\rho u^2 + \rho v^2) \right] (\gamma - 1) \tag{2.5}$$

The equation (2.5) is used to close the problem from the Euler's Equations and can be easily derived by considering that the total energy is the sum of internal and kinetic

energy. Observe that the internal energy e_i is given by $e_i = c_p T$, where c_p is the specific heat at constant pressure.

2.2.2 Differential Conservative Formulation

Again, the Gauss Theorem applied in the surface integrals leads to volume integrals with a divergent operator. This process allows one to write these set of equations in a differential formulation:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) &= 0 \\ \frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \otimes \vec{v} + p \vec{I}) &= \rho \vec{f}_e \\ \frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho H \vec{v}) &= \rho \vec{f}_e \cdot \vec{v}\end{aligned}\tag{2.6}$$

Or in the Einstein notation:

$$\begin{aligned}\partial_0 \rho + \partial_i (\rho v_i) &= 0 \\ \partial_0 (\rho v_i) + \partial_j (\rho v_j v_i + p \delta_{ji}) &= 0 \\ \partial_0 \left(\rho \left(e + \frac{1}{2} v_j v_j \right) \right) + \partial_i \left(\rho v_i \left(e + \frac{1}{2} v_j v_j + \frac{p}{\rho} \right) \right) &= 0\end{aligned}\tag{2.7}$$

2.2.3 Quasi-Linear Formulation

In a cartesian coordinate system, one can define the vectors containing the conservative variables and the flux quantities:

$$\mathbf{Q} = [\rho, \rho u, \rho v, \rho w, \rho E]^T \tag{2.8}$$

$$\mathbf{E} = [\rho u, \rho u^2 + p, \rho uv, \rho uw, \rho u H]^T \tag{2.9}$$

$$\mathbf{F} = [\rho v, \rho uv, \rho v^2 + p, \rho vw, \rho v H]^T \tag{2.10}$$

$$\mathbf{G} = [\rho w, \rho uw, \rho vw, \rho w^2 + p, \rho w H]^T \tag{2.11}$$

On neglecting the source terms due to the external forces, the Euler Equations can be written in a compact way as:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial y} + \frac{\partial \mathbf{G}}{\partial z} = 0 \tag{2.12}$$

Notice that it is a first order equation with respect to the conservative variables. In its quasi-linear form:

$$\frac{\partial \mathbf{Q}}{\partial t} + \left(\frac{\partial \vec{\mathbf{F}}}{\partial \mathbf{Q}} \right) \cdot \vec{\nabla} \mathbf{Q} = 0 \quad (2.13)$$

The vectors $\mathbf{E}$, $\mathbf{F}$ and $\mathbf{G}$ are the components of the flux-tensor $\vec{\mathbf{F}}$. In other words:

$$\frac{\partial \mathbf{Q}}{\partial t} + \underbrace{\frac{\partial \mathbf{E}}{\partial \mathbf{Q}}}_{\mathbf{A}} \frac{\partial \mathbf{Q}}{\partial x} + \underbrace{\frac{\partial \mathbf{F}}{\partial \mathbf{Q}}}_{\mathbf{B}} \frac{\partial \mathbf{Q}}{\partial y} + \underbrace{\frac{\partial \mathbf{G}}{\partial \mathbf{Q}}}_{\mathbf{C}} \frac{\partial \mathbf{Q}}{\partial z} = 0 \quad (2.14)$$

The matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are the flux jacobian matrices can be condensed as the components of the tensor $\vec{\mathbf{A}}$, defined as:

$$\vec{\mathbf{A}} = \frac{\partial \vec{\mathbf{F}}}{\partial \mathbf{Q}} \quad (2.15)$$

The flux-tensor is homogeneous of degree one with respect to the vector containing the conservative variables when the fluid satisfies the relation:

$$p = \rho f(e) \quad (2.16)$$

As one can notice, a perfect gas model is a particular case of the relation above. Because of the homogeneous property, one has the exact result:

$$\vec{\mathbf{F}}(\mathbf{Q}) = \frac{\partial \vec{\mathbf{F}}}{\partial \mathbf{Q}} \mathbf{Q} \implies \vec{\mathbf{F}}(\mathbf{Q}) = \vec{\mathbf{A}} \mathbf{Q} \quad (2.17)$$

Or in each component:

$$\mathbf{E} = \mathbf{A} \mathbf{Q} \quad \mathbf{F} = \mathbf{B} \mathbf{Q} \quad \mathbf{G} = \mathbf{C} \mathbf{Q} \quad (2.18)$$

The jacobian matrices are:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ -u^2 + \frac{\gamma-1}{2}\vec{v}^2 & (3-\gamma)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 \\ -uv & v & u & 0 & 0 \\ -uw & w & 0 & u & 0 \\ -u[\gamma E - (\gamma-1)\vec{v}^2] & \gamma E - \frac{\gamma-1}{2}(\vec{v}^2 + 2u^2) & -(\gamma-1)uv & -(\gamma-1)uw & \gamma u \end{bmatrix} \quad (2.19)$$

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ -uv & v & u & 0 & 0 \\ -v^2 + \frac{\gamma-1}{2}\vec{v}^2 & -(\gamma-1)v & (3-\gamma)u & -(\gamma-1)w & \gamma-1 \\ -vw & 0 & w & v & 0 \\ -v[\gamma E - (\gamma-1)\vec{v}^2] & -(\gamma-1)uv & \gamma E - \frac{\gamma-1}{2}(\vec{v}^2 + 2v^2) & -(\gamma-1)vw & \gamma v \end{bmatrix} \quad (2.20)$$

$$\mathbf{C} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ -uw & w & 0 & u & 0 \\ -vw & 0 & w & v & 0 \\ -w^2 + \frac{\gamma-1}{2}\vec{v}^2 & -(\gamma-1)u & -(\gamma-1)v & (3-\gamma)w & \gamma-1 \\ -w[\gamma E - (\gamma-1)\vec{v}^2] & -(\gamma-1)uw & -(\gamma-1)vw & \gamma E - \frac{\gamma-1}{2}(\vec{v}^2 + 2w^2) & \gamma w \end{bmatrix} \quad (2.21)$$

In order to simplify the matrices to make the process of obtaining the eigenvalues of the system easier, the Euler Equations are written as functions of the primitive variables $(\rho, \vec{v}, p)$ in a non-conservative form. In that case, the vector containing the primitive variables is defined by:

$$\mathbf{V} = [\rho, u, v, w, p]^T \quad (2.22)$$

And the system (2.14) becomes:

$$\frac{\partial \mathbf{V}}{\partial t} + \tilde{\mathbf{A}} \frac{\partial \mathbf{V}}{\partial x} + \tilde{\mathbf{B}} \frac{\partial \mathbf{V}}{\partial y} + \tilde{\mathbf{C}} \frac{\partial \mathbf{V}}{\partial z} = 0 \quad (2.23)$$

Where:

$$\begin{aligned}
\tilde{\mathbf{A}} &= \begin{bmatrix} u & \rho & 0 & 0 & 0 \\ 0 & u & 0 & 0 & \frac{1}{\rho} \\ 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & \gamma p & 0 & 0 & u \end{bmatrix} & \tilde{\mathbf{B}} &= \begin{bmatrix} v & 0 & \rho & 0 & 0 \\ 0 & v & 0 & 0 & 0 \\ 0 & 0 & v & 0 & \frac{1}{\rho} \\ 0 & 0 & 0 & v & 0 \\ 0 & 0 & \gamma p & 0 & v \end{bmatrix} & \tilde{\mathbf{C}} &= \begin{bmatrix} w & 0 & 0 & \rho & 0 \\ 0 & w & 0 & 0 & 0 \\ 0 & 0 & w & 0 & 0 \\ 0 & 0 & 0 & w & \frac{1}{\rho} \\ 0 & 0 & 0 & \gamma p & w \end{bmatrix}
\end{aligned} \tag{2.24}$$

The transformation matrix between the conservative and the non-conservative is only defined in terms of differentials and is given by:

$$\mathbf{M} = \frac{\partial \mathbf{Q}}{\partial \mathbf{V}} = \left(\frac{\partial \mathbf{U}}{\partial \rho} \quad \frac{\partial \mathbf{U}}{\partial \vec{v}} \quad \frac{\partial \mathbf{U}}{\partial p} \right) \tag{2.25}$$

Assuming a perfect gas model, the transformation jacobian matrix can be written explicitly as:

$$\mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ u & \rho & 0 & 0 & 0 \\ v & 0 & \rho & 0 & 0 \\ w & 0 & 0 & \rho & 0 \\ \frac{\vec{v}^2}{2} & \rho u & \rho v & \rho w & \frac{1}{\gamma-1} \end{bmatrix} \tag{2.26}$$

The relations between the jacobian matrices (2.19) and (2.24) are:

$$\begin{aligned}
\vec{\tilde{\mathbf{A}}} &= \mathbf{M}^{-1} \vec{\mathbf{A}} \mathbf{M} \\
\vec{\mathbf{A}} &= \mathbf{M} \vec{\tilde{\mathbf{A}}} \mathbf{M}^{-1}
\end{aligned} \tag{2.27}$$

2.2.4 Characteristic Form of the Euler's Equations

Now, consider the matrix defined by:

$$\mathbf{K} = \vec{k} \cdot \vec{\mathbf{A}} = k_x \mathbf{A} + k_y \mathbf{B} + k_z \mathbf{C} \tag{2.28}$$

$\mathbf{K}$ represents a projection of $\vec{\mathbf{A}}$ in the direction of the vector $\vec{k}$. The transformed tensor $\mathbf{K}$ in primitive variables is given by:

$$\tilde{\mathbf{K}} = \mathbf{M}^{-1}\mathbf{K}\mathbf{M} \quad (2.29)$$

As the Euler's equations are hyperbolic, the solutions are simple wave-like that have the form:

$$\mathbf{V} = \hat{\mathbf{V}} e^{iS(\vec{x},t)} = \hat{\mathbf{V}} e^{i(\vec{k}\cdot\vec{x}-\omega t)} \quad \text{where } i^2 = -1 \quad (2.30)$$

The $S(\vec{x}, t)$ function is the phase of a wave with pulsation ω travelling at the direction $\vec{k}$. This type of solution exists if the eigenvalues of $\tilde{\mathbf{K}}$ are real and linearly independent with the corresponding left eigenvector, for an arbitrary direction. One can define a matrix $\mathbf{L}^{-1}$ which can diagonalize $\tilde{\mathbf{K}}$, where each line j of $\mathbf{L}^{-1}$ corresponds to the j -th left eigenvector $\tilde{l}^j$:

$$\mathbf{L}^{-1} = \begin{bmatrix} k_x & 0 & k_z & -k_y & -\frac{k_x}{c^2} \\ k_y & -k_z & 0 & k_x & -\frac{k_y}{c^2} \\ k_z & k_y & -k_x & 0 & -\frac{k_z}{c^2} \\ 0 & k_x & k_y & k_z & \frac{1}{\rho c} \\ 0 & -k_x & -k_y & -k_z & \frac{1}{\rho c} \end{bmatrix} ; \quad \mathbf{L} = \begin{bmatrix} k_x & k_y & k_z & \frac{\rho}{2c} & \frac{\rho}{2c} \\ 0 & -k_z & k_y & \frac{k_x}{2} & -\frac{k_x}{2} \\ k_z & 0 & -k_x & \frac{k_y}{2} & -\frac{k_y}{2} \\ -k_y & k_x & 0 & \frac{k_z}{2} & -\frac{k_z}{2} \\ 0 & 0 & 0 & \frac{\rho c}{2} & \frac{\rho c}{2} \end{bmatrix} \quad (2.31)$$

And:

$$\mathbf{\Lambda} = \mathbf{L}^{-1}\tilde{\mathbf{K}}\mathbf{L} = \underbrace{\mathbf{L}^{-1}\mathbf{M}^{-1}}_{\mathbf{P}^{-1}} \mathbf{K} \underbrace{\mathbf{M}\mathbf{L}}_{\mathbf{P}} \quad (2.32)$$

$$\mathbf{\Lambda} = \begin{bmatrix} \vec{v} \cdot \vec{k} & 0 & 0 & 0 & 0 \\ 0 & \vec{v} \cdot \vec{k} & 0 & 0 & 0 \\ 0 & 0 & \vec{v} \cdot \vec{k} & 0 & 0 \\ 0 & 0 & 0 & \vec{v} \cdot \vec{k} + ck & 0 \\ 0 & 0 & 0 & 0 & \vec{v} \cdot \vec{k} - ck \end{bmatrix} \quad (2.33)$$

So the equation (2.23) can be manipulated:

$$\begin{aligned}
& \mathbf{L}^{-1} \frac{\partial \mathbf{V}}{\partial t} + \mathbf{L}^{-1} \tilde{\mathbf{A}} \frac{\partial \mathbf{V}}{\partial x} + \mathbf{L}^{-1} \tilde{\mathbf{B}} \frac{\partial \mathbf{V}}{\partial y} + \mathbf{L}^{-1} \tilde{\mathbf{C}} \frac{\partial \mathbf{V}}{\partial z} = 0 \Leftrightarrow \\
& \mathbf{L}^{-1} \frac{\partial \mathbf{V}}{\partial t} + \mathbf{L}^{-1} \tilde{\mathbf{A}} \mathbf{L} \mathbf{L}^{-1} \frac{\partial \mathbf{V}}{\partial x} + \mathbf{L}^{-1} \tilde{\mathbf{B}} \mathbf{L} \mathbf{L}^{-1} \frac{\partial \mathbf{V}}{\partial y} + \mathbf{L}^{-1} \tilde{\mathbf{C}} \mathbf{L} \mathbf{L}^{-1} \frac{\partial \mathbf{V}}{\partial z} = 0 \Leftrightarrow \\
& \frac{\partial \mathbf{W}}{\partial t} + \mathbf{L}^{-1} \tilde{\mathbf{A}} \mathbf{L} \frac{\partial \mathbf{W}}{\partial x} + \mathbf{L}^{-1} \tilde{\mathbf{B}} \mathbf{L} \frac{\partial \mathbf{W}}{\partial y} + \mathbf{L}^{-1} \tilde{\mathbf{C}} \mathbf{L} \frac{\partial \mathbf{W}}{\partial z} = 0
\end{aligned} \tag{2.34}$$

Or:

$$\frac{\partial \mathbf{W}}{\partial t} + \left(\mathbf{L}^{-1} \tilde{\mathbf{A}} \mathbf{L} \right) \cdot \vec{\nabla} \mathbf{W} = 0 \tag{2.35}$$

Where a new set of variables is introduced as:

$$\begin{aligned}
& \delta \mathbf{W} = \mathbf{L}^{-1} \delta \mathbf{V} \quad \text{or, in index form, } \delta w_k = \tilde{l}_i^k \delta v_i \\
& \text{and} \\
& \delta \mathbf{V} = \mathbf{L} \delta \mathbf{W}
\end{aligned} \tag{2.36}$$

The five elements of the column vector $\delta \mathbf{W}$ are called characteristic variables and are defined by their arbitrary variations. Each of the characteristic variables are associated with a direction of propagation $\vec{k}$.

$$\delta \mathbf{W} = [\delta w_1, \delta w_2, \delta w_3, \delta w_4]^T \tag{2.37}$$

$$\begin{aligned}
\delta w_1 &= \delta \rho - \frac{1}{c^2} \delta p \\
\delta w_2 &= k_x \delta w - k_z \delta u \\
\delta w_3 &= k_y \delta u - k_x \delta v \\
\delta w_4 &= \frac{1}{\rho c} \delta p + (k_x \delta u + k_y \delta v + k_z \delta w) \\
\delta w_5 &= \frac{1}{\rho c} \delta p - (k_x \delta u + k_y \delta v + k_z \delta w)
\end{aligned} \tag{2.38}$$

One can attribute a physical interpretation for each of the variables presented as explained by Hirsch (1988) [34]. The variable δw_1 is associated to the entropy perturbations; δw_2 and δw_3 are related to shear layer or vorticity waves in the characteristic surface which is normal to $\vec{k}$ (the direction of propagation); finally, δw_4 and δw_5 are connected to pressure waves.

2.2.5 Non-Dimensional Euler's Equations

The code originally developed by Hayashi (2006) [35] and used in this work makes use of non-dimensional variables defined as follows:

$$\begin{aligned} \rho^+ &= \frac{\rho}{\rho_\infty} & l^+ &= \frac{l}{l_0} & u_i^+ &= \frac{u_i}{c_\infty} & p^+ &= \frac{p}{\rho_\infty c_\infty^2} \\ t^+ &= \frac{c_\infty}{l_0} t & T^+ &= \frac{T}{T_\infty} & e^+ &= \frac{e}{\rho_\infty c_\infty^2} \end{aligned} \quad (2.39)$$

Where the subscript ∞ is related to properties computed at the non-perturbed flow and l_0 is a characteristic length.

By substitution of the above dimensionless variables for their dimensional counterparts in the Euler's Equations (2.12) and doing the proper simplifications, one has the dimensionless equations:

$$\frac{\partial \mathbf{Q}^+}{\partial t^+} + \frac{\partial \mathbf{E}^+}{\partial x^+} + \frac{\partial \mathbf{F}^+}{\partial y^+} + \frac{\partial \mathbf{G}^+}{\partial z^+} = 0 \quad (2.40)$$

Where:

$$\mathbf{Q}^+ = [\rho^+, \rho^+ u^+, \rho^+ v^+, \rho^+ w^+, \rho^+ E^+]^T \quad (2.41)$$

$$\mathbf{E}^+ = [\rho^+ u^+, \rho^+ u^{+2} + p^+, \rho^+ u^+ v^+, \rho^+ u^+ w^+, (e^+ + p^+) u^+]^T \quad (2.42)$$

$$\mathbf{F}^+ = [\rho^+ v^+, \rho^+ u^+ v^+, \rho^+ v^{+2} + p^+, \rho^+ v^+ w^+, (e^+ + p^+) v^+]^T \quad (2.43)$$

$$\mathbf{G}^+ = [\rho^+ w^+, \rho^+ u^+ w^+, \rho^+ v^+ w^+, \rho^+ w^{+2} + p^+, (e^+ + p^+) w^+]^T \quad (2.44)$$

From here on the variables are written in dimensionless form. To simplify the notation, the superscript $+$ is suppressed. An important note from Hayashi (2009) [35] is that these dimensionless variables are better suited for compressible flows. Otherwise, a more appropriate reference state should be chosen.

2.2.6 Euler's Equations in Generalized Coordinates

The Euler's Equations are usually presented in the literature in one of the two following forms: the extended form, which employs the general differential operators, and the reduced form, which associates the Cartesian to a transformed system of coordinates by a transformation operator (Volpe, 2013) [36]. A particular attention is given to the latter

one.

The development proposed in the previous sections is described in Cartesian coordinates, however, adopting a generalized coordinates system provides a more wide-range formulation, which, in this case, is convenient for the study of the control theory applied to the Euler's Equations.

An important fact to be highlighted is the choice of an appropriate transformation operator, that means, a transformed space where the specifications of the boundary conditions can be easily described.

The starting point is to assume that the flow domain is given in Cartesian coordinates. The transformation operator to the transformed space is denoted β and its inverse β^{-1} .

$$\underbrace{(x^{j'}, t)}_{\text{Flow domain}} \xrightleftharpoons[\beta^{-1}]{\beta} \underbrace{(\xi^i, t)}_{\text{Transformed space}}$$

The prime superscripts are used to represent Cartesian coordinates while unprimed indices refer to a transformed space. The transformation operators are defined as:

$$\begin{cases} \beta & \Rightarrow \beta_{j'}^i = \frac{\partial \xi^i}{\partial x^{j'}} : u^i = \beta_{j'}^i u^{j'} \\ \beta^{-1} & \Rightarrow \beta_i^{j'} = \frac{\partial x^{j'}}{\partial \xi^i} : u^{j'} = \beta_i^{j'} u^i \end{cases} \quad (2.45)$$

The transformation Jacobian is $J = \det(\beta_i^{j'})$. The Euler's Equations are written in index notation, according to the Cartesian coordinates:

$$\frac{\partial Q_\alpha}{\partial t} + \frac{\partial f_\alpha^{k'}}{\partial x^{k'}} = 0 \quad (2.46)$$

Where:

$$Q_\alpha \Rightarrow \left(\frac{\rho}{\rho u^{i'}} \right) ; f_\alpha^{k'} \Rightarrow \left(\frac{\rho u^{k'}}{\rho u^{i'k'} + p g^{i'k'}} \right) \quad (2.47)$$

Notice that the α index assumes the values 1 to 5 if considered a three dimensional space and 1 to 4 if bi-dimensional. The $\alpha = 1$ equation represents the continuity, for $1 < \alpha < n + 2$ (where n is the number of spacial dimensions) one has the momentum

equations and the equation represented when $\alpha = n + 2$ is the energy conservation.

In a transformed space, the Euler's Equations are:

$$J \frac{\partial Q_\alpha}{\partial t} + J \beta_{i'}^k \frac{\partial f_\alpha^{i'}}{\partial x^{k'}} = 0 \quad (2.48)$$

And if it is assumed that the Jacobian does not change in time and $\frac{(\partial J \beta_{i'}^k)}{\partial x^{k'}} = 0$:

$$\frac{\partial (J Q_\alpha)}{\partial t} + \frac{\partial F_\alpha^k}{\partial \xi^k} = 0 \quad (2.49)$$

Where the transformed flux vector F_α^k is:

$$F_\alpha^k = J \beta_{i'}^k f_\alpha^{i'} \quad (2.50)$$

It is convenient to write the equations based on the state vector Q_α , so defining a matrix $C_{\alpha\beta}^k$ as:

$$C_{\alpha\beta}^k = J \beta_{i'}^k \frac{\partial f_\alpha^{i'}}{\partial Q_\beta} = J \beta_{i'}^k A_{\alpha\beta}^{i'} \quad (2.51)$$

Finally, one can formulate the generalized Euler's Equations as:

$$\frac{\partial Q_\alpha}{\partial t} + \frac{C_{\alpha\beta}^k}{J} \frac{\partial Q_\beta}{\partial \xi^k} = 0 \quad (2.52)$$

3 NUMERICAL METHOD: PHYSICAL PROBLEM

As the present dissertation continues the work of Hayashi (2016) [33], the code to solve the partial differential equations is the one developed and validated (for steady-state flows) by the cited author. Since the objective is to extend the theory to unsteady or time-dependent flows, different features are added to the original code, however, the main methods of discretization are still the same found in Hayashi (2009 [35] and 2016 [33]).

In this chapter, the numerical approach to solve the Euler's Equations is described. The method was originated by Jameson, Schmidt and Turkel (1981) [37] and it is presented in this chapter. The spatial discretization used, namely the finite volume method, which allows the transformation of the partial differential equations into semi-discrete ordinary differential equations is presented. The ODE's can, then, be integrated in time by a Runge-Kutta scheme. The method uses an artificial dissipation term, which is explained in the next sections. Finally, the treatment of the boundary conditions using the characteristics Euler's Equations is explained.

3.1 Spatial Discretization

The Euler's Equations being PDE's, functions of time and space, are discretized in two steps: first in space and then in time. The spatial discretization is made via the finite volume method and allows one to transform the given PDE in a semi-discrete equation, which can be treated as an ODE in time.

3.1.1 Finite Volume Method

The rationale behind the Finite Volume Method is to discretize the conservative laws in their integral formulation. Alternatively, the technique can be classified as a finite difference method applied to the differential form of the conservative laws as highlighted by Hirsch (1988) [38]. A fundamental property of the method is the fact that it conserves

the mass, momentum and energy at the discrete level.

Consider the conservative law written for a discrete volume Ω , neglecting any source term:

$$\frac{\partial}{\partial t} \int_{\Omega} \mathbf{Q} d\Omega + \oint_S \vec{\mathbf{F}} \cdot d\vec{S} = 0 \quad (3.1)$$

Where $\mathbf{Q}$ is the vector containing the conservative variables and $\vec{\mathbf{F}}$ is the flux vector. The discretized equation is simply:

$$\frac{\partial}{\partial t} (\mathbf{Q}_i \Omega_i) + \sum_{sides} (\vec{\mathbf{F}} \cdot \vec{S}) = 0 \quad (3.2)$$

The second term in equation (3.2) is the sum of the fluxes at all sides of the control volume. $\mathbf{Q}_i$ represents the conservative quantities in the interior of Ω , which can be given by their corresponding averages in the volume Ω_i . One of the challenges when working with this method is to define an approximation to the volume Ω_i , its cell faces areas and the flux vector.

For the present purposes a 2D formulation is derived considering an unstructured mesh with triangular elements and properties initially defined at the center of the elements. That being said, the following approximation for $\mathbf{Q}_i$ is made (in Cartesian's coordinates):

$$\mathbf{Q}_i = \frac{1}{\Omega_i} \int_{\Omega_i} \mathbf{Q} dx dy \quad (3.3)$$

Now, in order to compute the cell face areas (lengths) and volume (area), one can consider the scheme of a control volume in figure 1.

The cell face lengths are:

$$\begin{aligned} \vec{S}_{AB} &= (y_B - y_A) \vec{e}_x - (x_B - x_A) \vec{e}_y \\ \vec{S}_{BC} &= (y_C - y_B) \vec{e}_x - (x_C - x_B) \vec{e}_y \end{aligned} \quad (3.4)$$

Where x and y are coordinates while $\vec{e}_x$ and $\vec{e}_y$ are unit vectors at directions x and y . The area of the control volume is:

$$\Omega_{ABC} = \frac{1}{2} \left| \vec{S}_{AB} \times \vec{S}_{BC} \right| \quad (3.5)$$

Figure 1: Cell centered triangular mesh

To compute the flux vectors in a bi-dimensional space, it is interesting to work with equation (3.1) written as:

$$\frac{\partial}{\partial t} \int_{\Omega} \mathbf{Q} d\Omega + \oint_S (\mathbf{E} dy - \mathbf{F} dx) = 0 \quad (3.6)$$

Where the vector $\vec{\mathbf{F}}$ was decomposed in its components $\vec{\mathbf{F}} = \mathbf{E}\vec{e}_x + \mathbf{F}\vec{e}_y$. The approximation for the fluxes to a triangular cell is then (Azevedo, 2006) [39]:

$$\oint_S (\mathbf{E} dy - \mathbf{F} dx) \approx \sum_{k=1}^3 [\mathbf{E}(\mathbf{Q}_{ik}) \Delta y_{ik} - \mathbf{F}(\mathbf{Q}_{ik}) \Delta x_{ik}] \quad (3.7)$$

With:

$$\mathbf{Q}_{ik} = \frac{1}{2} (\mathbf{Q}_i + \mathbf{Q}_k) \quad (3.8)$$

The surface integral approximated by equation (3.7) is the convective operator, usually represented by $C(\mathbf{Q}_i)$. Equation (3.1) becomes:

$$\frac{\partial (\mathbf{Q}_i \Omega_i)}{\partial t} + C(\mathbf{Q}_i) = 0 \quad (3.9)$$

3.1.2 Artificial Dissipation

The discretized equation (3.9) needs to be expanded by the addition of an artificial dissipation. As was discussed by Jameson, Schmidt and Turkel (1981) [37], it has been proven necessary to avoid the odd and even point decoupling and to prevent the appearance of wiggles in regions where the flow is submitted by a high pressure gradient, or in the neighborhood of stagnation points.

As explained in Hayashi (2009) [35], the capacity of the numerical solution to capture different frequencies is limited by the sizes of the elements. A typical example is a discontinuity in the flow, which has infinity modes and, thus, the high frequencies will not be detectable due to the finite mesh size (Pulliam, 1985) [40]. In real flows, the viscosity is the dissipation factor which limits the mode with high frequency. Although numerical dissipation always exists, as the Euler Equations are inviscid, an artificial dissipation mechanism is also added.

Some numerical methods add naturally dissipation factors in the discretization process, for example, when expanding determined terms in Taylor Series. One can also implement an artificial dissipation algorithm. Clearly, when non-physical dissipation is used, the user has to control it with caution (Hayashi, 2009) [35].

In this work, as the basis algorithm used is the one developed by Hayashi (2009 [35] and 2016 [33]), the artificial dissipation is added to equation (3.9) using the technique based on the work from Azevedo and Dourado (1991) [41] proposed by Jameson, Schmidt and Turkel (1981) [37]:

$$\frac{\partial (\mathbf{Q}_i \Omega_i)}{\partial t} + \underbrace{C(\mathbf{Q}_i)}_{\text{Convective}} - \underbrace{D(\mathbf{Q}_i)}_{\text{Dissipative}} = 0 \quad (3.10)$$

Where $D(\mathbf{Q}_i)$ is the operator representing the artificial dissipation and it can be split into two components:

$$D(\mathbf{Q}_i) = d^{(2)}(\mathbf{Q}_i) + d^{(4)}(\mathbf{Q}_i) \quad (3.11)$$

The first component represents a second difference defined by:

$$d^{(2)}(\mathbf{Q}_i) = \sum_k \left[\frac{1}{2} (A_i + A_k) \epsilon_{ik}^{(2)} (\mathbf{Q}_k - \mathbf{Q}_i) \right] \quad (3.12)$$

Where:

$$\begin{aligned} \epsilon_{ik}^{(2)} &= k^{(2)} \max(\nu_i, \nu_k) \quad \text{with} \quad k^{(2)} = \frac{1}{4} \\ \text{and} \\ \nu_i &= \frac{\sum_k |p_k - p_i|}{\sum_k (p_k + p_i)} \end{aligned} \tag{3.13}$$

And the term A_i is:

$$A_i = \sum_k \left[\left| \vec{v}_{ik} \cdot \vec{S}_{ik} \right| + a_{ik} \left| \vec{S}_{ik} \right| \right] \tag{3.14}$$

The second component of the dissipative term in equation (3.11) represents a fourth difference defined by:

$$d^{(4)}(\mathbf{Q}_i) = \sum_k \left[\frac{1}{2} (A_i + A_k) \epsilon_{ik}^{(4)} (\nabla^2 \mathbf{Q}_k - \nabla^2 \mathbf{Q}_i) \right] \tag{3.15}$$

Where:

$$\begin{aligned} \epsilon_{ik}^{(4)} &= \max \left[0, \left(k^{(4)} - \epsilon_{ik}^{(2)} \right) \right] \quad \text{with} \quad k^{(4)} = \frac{3}{256} \\ \text{and} \\ \nabla^2 \mathbf{Q}_i &= \sum_k (\mathbf{Q}_k - \mathbf{Q}_i) \end{aligned} \tag{3.16}$$

The term $d^{(2)}(\mathbf{Q}_i)$ increases the stability at discontinuities while the term $d^{(4)}(\mathbf{Q}_i)$ work at the smooth regions of the flow (Hayashi, 2009) [35]. The coefficients $k^{(2)}$ and $k^{(4)}$ are the ones used in Jameson, Schmidt and Turkel (1981) [37].

After the spatial discretization presented, equation (3.10) becomes an ordinary differential equation in time:

$$\frac{\partial (\mathbf{Q}_i \Omega_i)}{\partial t} + C(\mathbf{Q}_i) - D(\mathbf{Q}_i) = 0 \Rightarrow \frac{d\mathbf{Q}_i}{dt} = -\frac{1}{\Omega_i} [C(\mathbf{Q}_i) - D(\mathbf{Q}_i)] \tag{3.17}$$

3.2 Time Integration

Once the partial differential equations are discretized in space and, then, converted to an ordinary differential equations in time, usual numerical methods to solve ODE's

can be applied. The method already existent in the original code from Hayashi (2009) [35] for the time integration is the Runge-Kutta of 5 steps and second-order precision. However, differently from the cited work (which used a pseudo-time marching for a faster convergence to a steady solution), the present research consists in a time-accurate analysis of the flow, thus, some cautions have to be taken to guarantee a physical solution (for example, a same time step for all the elements).

The method is represented below:

$$\begin{aligned}
\mathbf{Q}_i^{(0)} &= \mathbf{Q}_i^{(n)} \\
\mathbf{Q}_i^{(1)} &= \mathbf{Q}_i^{(0)} - \alpha_1 \frac{\Delta t}{\Omega_i} \left[C \left(\mathbf{Q}_i^{(0)} \right) - D \left(\mathbf{Q}_i^{(0)} \right) \right] \\
\mathbf{Q}_i^{(2)} &= \mathbf{Q}_i^{(0)} - \alpha_2 \frac{\Delta t}{\Omega_i} \left[C \left(\mathbf{Q}_i^{(1)} \right) - D \left(\mathbf{Q}_i^{(1)} \right) \right] \\
\mathbf{Q}_i^{(3)} &= \mathbf{Q}_i^{(0)} - \alpha_3 \frac{\Delta t}{\Omega_i} \left[C \left(\mathbf{Q}_i^{(2)} \right) - D \left(\mathbf{Q}_i^{(1)} \right) \right] \\
\mathbf{Q}_i^{(4)} &= \mathbf{Q}_i^{(0)} - \alpha_4 \frac{\Delta t}{\Omega_i} \left[C \left(\mathbf{Q}_i^{(3)} \right) - D \left(\mathbf{Q}_i^{(1)} \right) \right] \\
\mathbf{Q}_i^{(5)} &= \mathbf{Q}_i^{(0)} - \alpha_5 \frac{\Delta t}{\Omega_i} \left[C \left(\mathbf{Q}_i^{(4)} \right) - D \left(\mathbf{Q}_i^{(1)} \right) \right] \\
\mathbf{Q}_i^{(n+1)} &= \mathbf{Q}_i^{(5)}
\end{aligned} \tag{3.18}$$

Where the α_i 's are:

$$\alpha_1 = \frac{1}{4}, \alpha_2 = \frac{1}{6}, \alpha_3 = \frac{3}{8}, \alpha_4 = \frac{1}{2} \text{ and } \alpha_5 = 1 \tag{3.19}$$

3.3 Boundary Conditions

To solve a partial differential equation, one requires an important information: the boundary conditions. However, it is important to know how many physical conditions are needed and, also, which remaining variables are necessary to be defined at the boundaries such as the problem be well-posed. Besides, the conditions must be formulated and discretized considering the compatibility of the internal scheme.

Once the characteristic formulation of the Euler's equations were presented, one can interpret the solution as simple waves which propagate transporting information. This information corresponds to the characteristic variables, a combination of primitive and conservative variables of the flow, and the velocity in which each wave travels is directly associated to the eigenvalues of $\tilde{\mathbf{K}}$.

To understand which of the physical conditions must be imposed it is necessary to evaluate the characteristic surface direction of propagation at the boundaries. Only the variables transported in the characteristics that travel from the boundaries towards the interior of the domain can be freely imposed, while the remaining variables (which travel from the inside towards the outside of the domain) depend on the computed flow, since they are part of the solution. Numerically, to solve the discretized equations, information of all the variables are required at the boundaries and, therefore, to complete the problem, it is necessary additional information besides the physical conditions, these pieces of information are called numerical boundary conditions. The number of physical plus numerical conditions must be equal to the number of dependent variables.

The missing information at the boundaries can be found in association with the outgoing characteristics. The characteristic variables related to the domain incoming waves are imposed as physical boundary conditions and the characteristic equations of the other variables are added as numerical conditions. This methodology is called characteristic boundary method. The addition of the Riemann variables (or compatibility equations) to the physical boundary conditions completes the set of equations required to solve the boundary problem.

Imposed combinations of conservative or primitive variables lead to a well-posed problem if all the information on both incoming and outgoing variables can be recovered.

On returning to equation (2.35), the characteristic form of the Euler's Equations, one can simplify it to a 2D case:

$$\left\{ \begin{array}{l} \frac{\partial \rho}{\partial t} - \frac{1}{c^2} \frac{\partial p}{\partial t} = - \left(\frac{\partial p}{\partial x} - \frac{1}{c^2} \frac{\partial p}{\partial x} \right) u - \left(\frac{\partial p}{\partial y} - \frac{1}{c^2} \frac{\partial p}{\partial y} \right) v \\ k_y \frac{\partial u}{\partial t} - k_x \frac{\partial v}{\partial t} = \frac{1}{\rho} \left(k_x \frac{\partial p}{\partial y} - k_y \frac{\partial p}{\partial x} \right) - \left(k_y \frac{\partial u}{\partial x} - k_x \frac{\partial v}{\partial x} \right) u - \left(k_y \frac{\partial u}{\partial y} - k_x \frac{\partial v}{\partial y} \right) v \\ \frac{\partial p}{\partial t} + \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = - (u + k_x c) \frac{\partial p}{\partial x} - (v + k_y c) \frac{\partial p}{\partial y} + \\ \quad - \rho c \left[(k_x u + c) \frac{\partial u}{\partial x} + k_y u \frac{\partial v}{\partial x} \right] - \rho c \left[(k_y v + c) \frac{\partial v}{\partial y} + k_x v \frac{\partial u}{\partial y} \right] \\ \frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = - (u + k_x c) \frac{\partial p}{\partial x} - (v + k_y c) \frac{\partial p}{\partial y} + \\ \quad + \rho c \left[(k_x u + c) \frac{\partial u}{\partial x} + k_y u \frac{\partial v}{\partial x} \right] + \rho c \left[(k_y v + c) \frac{\partial v}{\partial y} + k_x v \frac{\partial u}{\partial y} \right] \end{array} \right. \quad (3.20)$$

If the right hand side of each equation is defined by R_i (which carries the spatial

derivatives) one gets:

$$\begin{cases} \frac{\partial \rho}{\partial t} - \frac{1}{c^2} \frac{\partial p}{\partial t} = R_1 \\ k_y \frac{\partial u}{\partial t} - k_x \frac{\partial v}{\partial t} = R_2 \\ \frac{\partial p}{\partial t} + \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_3 \\ \frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4 \end{cases} \quad (3.21)$$

And according to the information acquired from the eigenvalues determined in equation (2.33), for the bi-dimensional case:

$$\mathbf{\Lambda} = \begin{bmatrix} \vec{v} \cdot \vec{k} & 0 & 0 & 0 \\ 0 & \vec{v} \cdot \vec{k} & 0 & 0 \\ 0 & 0 & \vec{v} \cdot \vec{k} + ck & 0 \\ 0 & 0 & 0 & \vec{v} \cdot \vec{k} - ck \end{bmatrix} \quad (3.22)$$

As explained before, these eigenvalues are related to the characteristics velocities, indicating whether they are entering or leaving the domain. Thus, given a boundary, it is possible to determine how many characteristics are entering or leaving.

Nevertheless, some difficulties implementing the boundary conditions arise when using a cell centered scheme. Evidently, at the boundary, the cells do not have neighbours at all sides. The technique used to implement the boundary conditions was the so called ghost cells, which are not part of the physical domain but are adjacent to the cells at the contour of the domain. The properties inside the ghost cells do not need to be physically possible. All that is required of them is to impose the appropriate domain boundary conditions.

3.3.1 Inlet

At the inlet $\vec{v} \cdot \vec{k}$ and $\vec{v} \cdot \vec{k} + ck$ are always positive. Clearly, if the fluid is entering by that surface normal is positioned towards the interior of the domain, then, they have the same signal. However, the signal of the eigenvalue associated to $\vec{v} \cdot \vec{k} - ck$ relies on the magnitude of $\vec{v}$. If $v > c$ (supersonic inlet), it follows that the characteristic is entering the domain, but if $v < c$ (subsonic inlet), then the eigenvalue is negative and the characteristic is leaving the domain.

3.3.1.1 Subsonic

Table 1 summarizes the information used to solve the subsonic inlet condition:

Table 1: Physical and numerical conditions at the subsonic inlet

Characteristics entering the domain	3
Characteristics leaving the domain	1
Imposed physical conditions	$p_0 ; T_0 ; \alpha$
Numerical conditions/Compatibility relations	$\frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4$

The physical conditions imposed at the inlet are chosen to be the stagnation pressure, stagnation temperature and incident angle of the flow. This choice must be made carefully to guarantee a well-posed condition (Hirsch, 1994) [34]. The compatibility equation is the one associated to the characteristic which leaves the domain (fourth equation from (3.21)). With the information on table 1, the complete state in the ghost cells must be well determined.

The following approximation is made:

$$\frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4 \Rightarrow \delta p - \rho c (k_x \delta u + k_y \delta v) = \Delta t R_4 \quad (3.23)$$

With some algebra, from equation (3.23) it is possible to define the evolution of the ghost cells properties. The detailed development is made in Hayashi (2009) [35]. However, some assumptions made in the latter are highlighted at this work.

Considering an angle α , one has that $\frac{\delta u}{\delta v} = \frac{u}{v}$, besides it is assumed that $\delta p = \frac{\partial p}{\partial U} \delta U$. The derivative $\frac{\partial p}{\partial U}$ in the second relation can be obtained by the definition of stagnation pressure (which is one of the physical conditions imposed):

$$p_0 = p \left[1 - \frac{\gamma - 1}{\gamma + 1} \frac{u^2 + v^2}{a_\star^2} \right]^{-\frac{\gamma}{\gamma - 1}} \quad \text{with} \quad a_\star^2 = \frac{2\gamma T}{\gamma + 1} \quad (3.24)$$

With the proper manipulations and substitutions in equation (3.23), one has that:

$$\delta u = \frac{\Delta t R_4}{-\frac{p_0 \gamma M}{c} \left[1 + \frac{(\gamma-1)}{2} M^2 \right]^{\frac{1-2\gamma}{\gamma-1}} \left(\frac{u}{U} + \frac{v^2}{uU} \right) - \rho c \left(k_x + k_y \frac{v}{u} \right)} \quad (3.25)$$

With the relation $\frac{\delta u}{\delta v} = \frac{u}{v}$, δv is equally determined. Also, with definition (3.24) and definition of stagnation temperature (3.26), the evolution of all properties of the ghost cells are well determined.

$$T_0 = T \left[1 - \frac{\gamma-1}{\gamma+1} \frac{u^2 + v^2}{a_\star^2} \right]^{-1} \quad \text{with} \quad a_\star^2 = \frac{2\gamma T}{\gamma+1} \quad (3.26)$$

Given an inlet ghost cell, it follows that:

$$\begin{aligned} u_{ghost}^{n+1} &= u_{ghost}^n + \delta u \\ v_{ghost}^{n+1} &= v_{ghost}^n + \delta v \\ p_{ghost}^{n+1} &= p(u_{ghost}^{n+1}) \\ T_{ghost}^{n+1} &= T(u_{ghost}^{n+1}) \end{aligned} \quad (3.27)$$

Notice that, at the present approach, p_0 , T_0 and α at the inlet can vary in time according to the imposed functions $p_0(t)$, $T_0(t)$ and $\alpha(t)$. Nevertheless, the past equations holds, only with the caution that p_0 , T_0 and α can change from a time step to another.

3.3.1.2 Supersonic

The supersonic case is direct in the sense that all the characteristics enter the domain and, thus, all physical conditions are imposed, totally defining the ghost cells states at any time. Table 2 summarize the conditions:

Table 2: Physical and numerical conditions at the supersonic inlet

Characteristics entering the domain	4
Characteristics leaving the domain	0
Imposed physical conditions	$u ; v ; p ; T$
Numerical conditions/Compatibility relations	-

3.3.2 Outlet

At the outlet the normal vector to the the surface is always opposed to the velocity vector $\vec{v}$. From equation (2.33), the characteristic related to $\vec{v} \cdot \vec{k}$ and $\vec{v} \cdot \vec{k} - ck$ are always negative, meaning that the information being carried by them are leaving the domain. Again, one of the characteristics changes its sense according to the flow's regime (super or subsonic). When $v < c$ (subsonic), then $\vec{v} \cdot \vec{k} + ck$ is positive (characteristic enters the domain) and when $v > c$ (supersonic), then $\vec{v} \cdot \vec{k} + ck$ is negative (characteristic leaves the domain).

3.3.2.1 Subsonic

According to the exposed, table 3 shows the physical condition as well as the compatibility relations at the outlet:

Table 3: Physical and numerical conditions at the subsonic outlet

Characteristics entering the domain	1
Characteristics leaving the domain	3
Imposed physical conditions	p
Numerical conditions/Compatibility relations	$\frac{\partial \rho}{\partial t} - \frac{1}{c^2} \frac{\partial p}{\partial t} = R_1$ $k_y \frac{\partial u}{\partial t} - k_x \frac{\partial v}{\partial t} = R_2$ $\frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4$

As the inlet condition, the information summarized in the four conditions (one physical and three numerical) allows one to fully specify the ghost cells. The process is detailed in Hayashi (2009) [35], however, as the present case considers the time-dependent imposed pressure at the outlet, the term $\frac{\partial p}{\partial t}$ is not considered null.

The approximation made is:

$$\begin{cases} \frac{\partial \rho}{\partial t} - \frac{1}{c^2} \frac{\partial p}{\partial t} = R_1 \\ k_y \frac{\partial u}{\partial t} - k_x \frac{\partial v}{\partial t} = R_2 \\ \frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4 \end{cases} \Rightarrow \begin{cases} \delta \rho = \Delta t \left[R_1 + \frac{1}{c^2} \frac{\partial p}{\partial t} \right] \\ k_y \delta u - k_x \delta v = \Delta t R_2 \\ -\rho c (k_x \delta u + k_y \delta v) = \Delta t \left[R_4 - \frac{\partial p}{\partial t} \right] \end{cases} \quad (3.28)$$

Notice here that $\frac{\partial p}{\partial t}$ is known, as it is an imposed condition. The only difference between the treatment made in Hayashi (2009) [35] is that $p = p(t)$ is a function of time and not a fixed single value.

The evolution of p at the ghost cell is determined (once it is one of the imposed properties). From the first equation in (3.28), the evolution of ρ at the ghost cells can be calculated. Finally, from the second and third equations:

$$\text{if } k_y \neq 0 \quad \begin{cases} \delta v = - \left[k_x R_2 + \frac{k_y (R_4 - \frac{\partial p}{\partial t})}{\rho c} \right] \Delta t \\ \delta u = \frac{\Delta t R_2 - k_x \left[k_x R_2 + \frac{k_y (R_4 - \frac{\partial p}{\partial t})}{\rho c} \right] \Delta t}{k_y} \end{cases} \quad (3.29)$$

$$\text{if } k_y = 0 \text{ and } k_x = -1 \quad \begin{cases} \delta v = \Delta t R_2 \\ \delta u = \frac{\Delta t [R_4 - \frac{\partial p}{\partial t}]}{\rho c} \end{cases} \quad (3.30)$$

And the ghost cells properties are updated as following:

$$\begin{aligned} \rho_{ghost}^{n+1} &= \rho_{ghost}^n + \delta \rho \\ u_{ghost}^{n+1} &= u_{ghost}^n + \delta u \\ v_{ghost}^{n+1} &= v_{ghost}^n + \delta v \end{aligned} \quad (3.31)$$

3.3.2.2 Supersonic

A supersonic outlet has all the characteristics leaving the domain. In other words, all the information are propagated from the interior of the domain towards the exterior. Consequently, no physical conditions are imposed and the properties of the ghost cells are defined by the compatibility relations.

From the relations in table 4 and considering $\delta p = \frac{\partial p}{\partial t} \Delta t$ it comes that:

Table 4: Physical and numerical conditions at the supersonic outlet

Characteristics entering the domain	0
Characteristics leaving the domain	4
Imposed physical conditions	-
Numerical conditions/Compatibility relations	$\frac{\partial \rho}{\partial t} - \frac{1}{c^2} \frac{\partial p}{\partial t} = R_1$ $k_y \frac{\partial u}{\partial t} - k_x \frac{\partial v}{\partial t} = R_2$ $\frac{\partial p}{\partial t} + \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_3$ $\frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4$

$$\left\{ \begin{array}{l} \frac{\partial \rho}{\partial t} - \frac{1}{c^2} \frac{\partial p}{\partial t} = R_1 \\ k_y \frac{\partial u}{\partial t} - k_x \frac{\partial v}{\partial t} = R_2 \\ \frac{\partial p}{\partial t} + \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_3 \\ \frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4 \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \delta \rho = \Delta t R_1 + \frac{1}{c^2} \delta p \\ k_y \delta u - k_x \delta v = \Delta t R_2 \\ \rho c (k_x \delta u + k_y \delta v) = \Delta t R_3 - \delta p \\ -\rho c (k_x \delta u + k_y \delta v) = \Delta t R_4 - \delta p \end{array} \right. \quad (3.32)$$

Solving the system in $\delta \rho$, δp , δu and δv :

$$\delta p = \left(\frac{R_3 + R_4}{2} \right) \Delta t \quad (3.33)$$

$$\delta \rho = \Delta t R_1 + \frac{\delta p}{c^2} \quad (3.34)$$

$$\text{if } k_y \neq 0 \quad \left\{ \begin{array}{l} \delta v = \frac{k_y}{\rho c} (\delta p - \Delta t R_4) - k_x \Delta t R_2 \\ \delta u = \frac{\Delta t R_2 + k_x \left[\frac{k_y}{\rho c} (\delta p - \Delta t R_4) - k_x \Delta t R_2 \right] \Delta t}{k_y} \end{array} \right. \quad (3.35)$$

$$\text{if } k_y = 0 \text{ and } k_x = -1 \quad \left\{ \begin{array}{l} \delta v = \Delta t R_2 \\ \delta u = \frac{\Delta t R_4 - \delta p}{\rho c} \end{array} \right. \quad (3.36)$$

Having all the variations needed, the ghost cells properties are then:

$$\begin{aligned}
 \rho_{ghost}^{n+1} &= \rho_{ghost}^n + \delta\rho \\
 u_{ghost}^{n+1} &= u_{ghost}^n + \delta u \\
 v_{ghost}^{n+1} &= v_{ghost}^n + \delta v \\
 p_{ghost}^{n+1} &= p_{ghost}^n + \delta p
 \end{aligned} \tag{3.37}$$

3.3.3 Solid Wall

Since it is considered that no flux can cross the wall, meaning that the fluid can't penetrate the body. Only one eigenvalue is positive and, hence, one physical condition is imposed: the normal component of the velocity with respect to the surface must be null ($v_n = 0$). To define the variables at the ghost cells it is necessary to extrapolate the information from the interior of the domain with the fourth compatibility relation.

From the physical condition, the ghost cells velocities are:

$$\begin{aligned}
 v_{n,ghost} &= -v_n \\
 v_{t,ghost} &= v_t
 \end{aligned} \tag{3.38}$$

Where the normal velocity of the ghost cell $v_{n,ghost}$ must be equal to the v_n of the interior domain but with opposed signal, that way the normal velocity at the boundary is zero. On the other hand, the tangential components from both ghost and interior cell must be exactly the same.

It remains the information of the pressure at the ghost cells to be computed. It is done by solving the fourth characteristic equation:

$$\frac{\partial p}{\partial t} - \rho c \left(k_x \frac{\partial u}{\partial t} + k_y \frac{\partial v}{\partial t} \right) = R_4 \tag{3.39}$$

Again, the details of the development for obtaining the pressure condition are found by Hayashi (2009) [35]. The idea is to write the fourth compatibility relation with respect to the tangential and normal components of the velocity and to combine it with the continuity equation. With the assumption that the curvature radius of the solid wall R_w is great $R_w \gg 1$, it comes that the gradient of the static pressure at the solid wall is null. Hence:

$$p_{ghost} = p_{interior} \tag{3.40}$$

4 ADJOINT METHOD APPLIED TO THE EULER'S EQUATIONS

The aim of the present section is to establish the adjoint problem for compressible flows, modelled by the Euler Equations, using the general approach given by Cacuci (1980) [2] and extending the development found in Hayashi (2016) [33] and Hayashi, Ceze and Volpe (2018) [42] for time-dependent problems with both inlet and outlet control parameters conditions. To reach this objective, the variation of the augmented objective functional is obtained. The boundary conditions and the adjoint equation in its characteristic form are developed to compute the sensitivities of the cost functional with respect to the permeable boundaries properties.

4.1 Variation of the Augmented Objective Functional

The variational problem associated with a measure of merit restricted by the Euler's Equation is developed following the sensitivity theory for general systems of nonlinear equations formalised by (Cacuci et al., 1980), as described before.

In the context of this work, the objective functional is taken as a surface integral related to the aerodynamics forces. To construct the augmented objective functional, one shall starts from equation (1.29). The governing equations treated as constraints are the Euler's Equation, given in general coordinates as in equation (2.49). The functional is rewritten as:

$$G = \underbrace{\frac{1}{T} \int_{t_0}^{t_f} \int_{b_w} \mathcal{F}[\mathbf{Q}, \mathbf{P}] \left| \frac{dS'}{dS} \right| dS dt}_I + \underbrace{\left\langle \phi_\alpha, \frac{\partial (JQ_\alpha)}{\partial t} + \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle}_{I_1} + \underbrace{\langle \psi, \mathbf{B} \rangle_s}_{I_2} + \underbrace{\langle \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle}_{I_3} \quad (4.1)$$

The variation of the augmented functional is computed by taking the variation of each term. The first one, I , represents the cost functional considering the change of

coordinates. It can be written using the inner product defined in equations (1.28) and its first variation is given by:

$$\delta I = \left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right|, \delta Q_\alpha \right\rangle_{b_w} + \left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle_{b_w} \quad (4.2)$$

The term I_1 , related to the governing equations restriction, can be split into two inner products:

$$\delta I_1 = \underbrace{\delta \left\langle \phi_\alpha, \frac{\partial (JQ_\alpha)}{\partial t} \right\rangle}_{\delta I_{1a}} + \underbrace{\delta \left\langle \phi_\alpha, \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle}_{\delta I_{1b}} \quad (4.3)$$

The first variation of δI_{1a} is:

$$\delta \left\langle \phi_\alpha, \frac{\partial (JQ_\alpha)}{\partial t} \right\rangle = \left\langle \delta \phi_\alpha, \frac{\partial (JQ_\alpha)}{\partial t} \right\rangle + \left\langle \phi_\alpha, \frac{\partial (Q_\alpha \delta J)}{\partial t} \right\rangle + \left\langle \phi_\alpha, \frac{\partial (J \delta Q_\alpha)}{\partial t} \right\rangle \quad (4.4)$$

Integrating by parts the last term of equation (4.4), one finds:

$$\int_{t_0}^{t_f} \int_{\Omega} \phi_\alpha \frac{\partial (J \delta Q_\alpha)}{\partial t} d\Omega dt = \left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0}^{t_f} - \left\langle \frac{\partial \phi_\alpha}{\partial t}, (J \delta Q_\alpha) \right\rangle \quad (4.5)$$

The term δI_{1b} :

$$\delta \left\langle \phi_\alpha, \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle = \left\langle \delta \phi_\alpha, \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle + \left\langle \phi_\alpha, \frac{\partial (\delta F_\alpha^k)}{\partial \xi^k} \right\rangle \quad (4.6)$$

From the chain's rule, the following relation can be integrated:

$$\frac{\partial}{\partial \xi^k} (J \phi_\alpha \delta F_\alpha^k) = J \phi_\alpha \frac{\partial (\delta F_\alpha^k)}{\partial \xi^k} + \delta F_\alpha^k \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \quad (4.7)$$

Implying that:

$$\int_{t_0}^{t_f} \int_{\Omega} \frac{1}{J} \frac{\partial}{\partial \xi^k} (J \phi_\alpha \delta F_\alpha^k) d\Omega dt = \left\langle \phi_\alpha, \frac{\partial (\delta F_\alpha^k)}{\partial \xi^k} \right\rangle + \left\langle \frac{\delta F_\alpha^k}{J}, \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \right\rangle \quad (4.8)$$

In order to transform the domain integral into a surface integral, one can apply the Gauss Theorem in the LHS of equation (4.8):

$$\langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_s = \left\langle \phi_\alpha, \frac{\partial (\delta F_\alpha^k)}{\partial \xi^k} \right\rangle + \left\langle \frac{\delta F_\alpha^k}{J}, \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \right\rangle \quad (4.9)$$

The term δI_2 is the first variation of the constraint from boundary conditions and δI_3 is the variation due to change of parameters around a basis configuration:

$$\delta I_2 = \langle \delta \psi, \mathbf{B} \rangle_s + \langle \psi, \delta \mathbf{B} \rangle_s = \langle \delta \psi, \mathbf{B} \rangle_s + \langle \psi, \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_s + \langle \psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s \quad (4.10)$$

$$\delta I_3 = \langle \delta \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle + \langle \mathbf{a}, \delta \mathbf{P} \rangle \quad (4.11)$$

Replacing the variations δI , δI_1 , δI_2 and δI_3 in equation (4.1):

$$\begin{aligned} \delta G = & \underbrace{\left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right|, \delta Q_\alpha \right\rangle_{b_w}}_{\delta I} + \left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle_{b_w} + \\ & \underbrace{\left\langle \delta \phi_\alpha, \frac{\partial (J Q_\alpha)}{\partial t} \right\rangle + \left\langle \phi_\alpha, \frac{\partial (Q_\alpha \delta J)}{\partial t} \right\rangle + \left[\int_\Omega \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0}^{t_f} - \left\langle \frac{\partial \phi_\alpha}{\partial t}, (J \delta Q_\alpha) \right\rangle}_{\delta I_{1a}} + \\ & \underbrace{\left\langle \delta \phi_\alpha, \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle + \langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_s - \left\langle \frac{\delta F_\alpha^k}{J}, \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \right\rangle}_{\delta I_{1b}} \\ & \underbrace{\langle \delta \psi, \mathbf{B} \rangle_s + \langle \psi, \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_s + \langle \psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s}_{\delta I_2} + \\ & \underbrace{\langle \delta \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle + \langle \mathbf{a}, \delta \mathbf{P} \rangle}_{\delta I_3} \end{aligned} \quad (4.12)$$

The term of the surface integral (with subscript s) is the bilinear concomitant $P[\phi, \delta \mathbf{Q}]$. The versor n_k is normal to the boundaries and points to inside of the domain. The bilinear concomitant can be split conveniently, according to each control surface: inlet (s_i), outlet (s_o), body surface or rigid body (b_w) and plane cuts (b_{cp}):

$$\langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_s = \langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_{s_i} + \langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_{s_o} + \langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_{b_w} + \left[\langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_{b_{cp}} \right]_{b_{cp}^+}^{b_{cp}^-} \quad (4.13)$$

If imposed periodic boundary conditions on the plane cuts as $\phi_\alpha|_{b_{cp}^+} = \phi_\alpha|_{b_{cp}^-}$, the

integrals over these planes cancel each other once the normal versors have opposite signs.

As discussed previously in this work, the augmented cost functional assumes the governing equations and boundary conditions as constraints. However it is yet needed to ensure that one works inside the space of admissible flow solutions. An important physical condition is the absence of normal flux at the body surface. In other words, $u_i n_i = 0$ at b_w , consequently, the flux at this boundary and its first variation become:

$$F_\alpha^k \Big|_{\xi^2=0} = J^{-1} \begin{pmatrix} 0 \\ p \xi_x^2 \\ p \xi_y^2 \\ 0 \end{pmatrix} \Rightarrow \delta F_\alpha^k \Big|_{\xi^2=0} = J \begin{pmatrix} 0 \\ \delta p \xi_x^2 \\ \delta p \xi_y^2 \\ 0 \end{pmatrix} + p \begin{pmatrix} 0 \\ \delta (J \xi_x^2) \\ \delta (J \xi_y^2) \\ 0 \end{pmatrix} \quad (4.14)$$

It is convenient the use of a transformed space where the boundaries can be easily described. A common choice is a mapping that arrives from the flow domain to a rectangular domain, so the boundaries and their normal unit vectors are parallels to the axis. There the rigid wall corresponding to the body surface is mapped in the plane $\xi^2 = 0$. The product which appears in the term of the bilinear concomitant at the rigid wall is, then:

$$\begin{aligned} \phi_\alpha \delta F_\alpha^k n_k \Big|_{b_w \Rightarrow \xi^2=0} &= \delta p [\phi_{i'+1} J \beta_{i'}^2 n_2] + p [\phi_{i'+1} \delta (J \beta_{i'}^2) n_2] \Leftrightarrow \\ \langle \phi_\alpha, \delta F_\alpha^k n_k \rangle_{b_w \Rightarrow \xi^2=0} &= \langle \delta p, [\phi_{i'+1} J \beta_{i'}^2 n_2] \rangle + \langle p, [\phi_{i'+1} \delta (J \beta_{i'}^2) n_2] \rangle \end{aligned} \quad (4.15)$$

Again, the index α varies from 1 to $i' + 2$ and for the momentum equations α and i' are related simply by $\alpha = i' + 1$ (e. g., if in Cartesian coordinate, the equation with $\alpha = 3$ corresponds to the momentum equation in $x_{i'} = x_2 = y$, that is $i' = 2$). Finally, from equations (2.50) and (2.51):

$$\delta F_\alpha^k = C_{\alpha\beta}^k \delta Q_\beta + \delta (J \beta_{i'}^k) f_\alpha^{i'} \quad (4.16)$$

One can rewrite the augmented cost functional as:

$$\begin{aligned}
 \delta G = & \left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right| + \frac{\partial p}{\partial Q_\alpha} [\phi_{i'+1} J \beta_{i'}^2 n_2], \delta Q_\alpha \right\rangle_{b_w} + \left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle_{b_w} + \\
 & \left\langle \delta \phi_\alpha, \frac{\partial (J Q_\alpha)}{\partial t} \right\rangle + \left\langle \phi_\alpha, \frac{\partial (Q_\alpha \delta J)}{\partial t} \right\rangle + \left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0}^{t_f} - \left\langle \frac{\partial \phi_\alpha}{\partial t}, (J \delta Q_\alpha) \right\rangle + \\
 & \left\langle \delta \phi_\alpha, \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle + \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_i} + \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_o} + \\
 & \left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_i} + \left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_o} + \\
 & \langle p, [\phi_{i'+1} \delta (J \beta_{i'}^2) n_2] \rangle_{b_w} - \left\langle \frac{C_{\alpha\beta}^k}{J} \frac{\partial (J \phi_\alpha)}{\partial \xi^k}, \delta Q_\beta \right\rangle - \left\langle \delta (J \beta_{i'}^k), \frac{f_\alpha^{i'}}{J} \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \right\rangle \\
 & \langle \delta \psi, \mathbf{B} \rangle_s + \langle \psi, \mathbf{B}'_P \delta \mathbf{P} \rangle_s + \langle \delta \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle + \langle \mathbf{a}, \delta \mathbf{P} \rangle
 \end{aligned} \tag{4.17}$$

Or, on rearranging the terms:

$$\begin{aligned}
 \delta G = & \underbrace{\left\langle \delta \phi_\alpha, \frac{\partial (J Q_\alpha)}{\partial t} \right\rangle + \left\langle \delta \phi_\alpha, \frac{\partial F_\alpha^k}{\partial \xi^k} \right\rangle + \langle \delta \psi, \mathbf{B} \rangle_s + \langle \delta \mathbf{a}, \mathbf{P} - \mathbf{P}_0 \rangle +}_{\text{(I) Physical problem}} \\
 & \underbrace{- \left\langle \frac{\partial \phi_\alpha}{\partial t}, (J \delta Q_\alpha) \right\rangle - \left\langle \frac{C_{\alpha\beta}^k}{J} \frac{\partial (J \phi_\alpha)}{\partial \xi^k}, \delta Q_\beta \right\rangle +}_{\text{(II) Adjoint equation}} \\
 & \underbrace{\left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_i} + \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_o}}_{\text{(III) Adjoint boundary conditions}} + \\
 & \underbrace{\left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right| + \frac{\partial p}{\partial Q_\alpha} [\phi_{i'+1} J \beta_{i'}^2 n_2], \delta Q_\alpha \right\rangle_{b_w}}_{\text{(III) Adjoint boundary conditions}} + \underbrace{\left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0}^{t_f}}_{\text{(IV) Time condition}} + \\
 & \underbrace{\left[\left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_i} + \left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_o} \right]_{=\text{farfield}} + \left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle_{b_w}}_{\text{(V) Adjoint gradient}} + \\
 & \underbrace{\left\langle \phi_\alpha, \frac{\partial (Q_\alpha \delta J)}{\partial t} \right\rangle - \left\langle \delta (J \beta_{i'}^k), \frac{f_\alpha^{i'}}{J} \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \right\rangle + \langle p, [\phi_{i'+1} \delta (J \beta_{i'}^2) n_2] \rangle_{b_w}}_{\text{(V) Adjoint gradient}} + \\
 & \underbrace{\langle \psi, \mathbf{B}'_P \delta \mathbf{P} \rangle_s + \langle \mathbf{a}, \delta \mathbf{P} \rangle}_{\text{(V) Adjoint gradient}}
 \end{aligned} \tag{4.18}$$

The way it was written, different sets of terms can be seen, each of playing a certain role in the total variational problem. The set denoted by (I) represents the terms that

constitute the physical model (governing equations, boundary conditions and the difference to the reference configuration) inner product with the respective first variation of the Lagrange multipliers. The sets (II) and (III) are inner products with the physical variation $\delta\mathbf{Q}$, being part of the adjoint problem. Notice that (II) is an integral over the domain, defining the adjoint equations, while (III) represents surface integrals, defining the boundary adjoint conditions (respectively, inlet, outlet and body surface). The term (IV) completes the adjoint problem as a time condition. The remaining terms in (V) make part of the adjoint gradient. The surface integrals terms at the inlet s_i and outlet s_o that are not associated with $\delta\mathbf{Q}$ were regrouped as the farfield term ($s_i \cup s_o \Rightarrow b_\infty$). This boundary can be mapped on the constant plane $b_\infty \Rightarrow \xi^2 = 1$ at the transformed space, analogous to what was done for the rigid wall ($\xi^2 = 0$).

The aim is using the adjoint method is to eliminate the terms dependents to the physical variations so the gradient can be computed with just one base solution of the flow field. Solve the flow solution permits canceling automatically the set (I). One can then eliminate the terms in (II), (III) and (IV) on solving the adjoint equation, given the boundary and time conditions. Hence, on solving both the flow and adjoint problems, one is left with the terms in (V), only, to compute the gradient. The majority of the gradient terms can be neglected if the Jacobian is constant.

4.2 Adjoint Equation

The adjoint equation arises from (II) in equation (4.18):

$$(II) = - \left\langle \frac{\partial \phi_\alpha}{\partial t}, (J \delta Q_\alpha) \right\rangle - \left\langle \frac{C_{\alpha\beta}^k}{J} \frac{\partial (J \phi_\alpha)}{\partial \xi^k}, \delta Q_\beta \right\rangle = 0 \quad (4.19)$$

In order to drive (II) to zero for any physical variation in the state vector, one can impose:

$$\frac{\partial (J \phi_\alpha)}{\partial t} + \frac{C_{\beta\alpha}^k}{J} \frac{\partial (J \phi_\beta)}{\partial \xi^k} = 0 \quad (4.20)$$

It is necessary, though, that $\delta\mathbf{Q}$ be realizable and, in order to compute the gradient, ϕ must be non-trivial. Notice that the adjoint equation carries the matrix $C_{\beta\alpha}^k$, transpose of $C_{\alpha\beta}^k$, due to the index manipulation in the second term of expression (4.19). One can redefine the adjoint variable so as to incorporate the transformation Jacobian $\varphi_\alpha = J \phi_\alpha$. It leads to the final expression of the adjoint equation:

$$\frac{\partial \varphi_\alpha}{\partial t} + \frac{C_{\beta\alpha}^k}{J} \frac{\partial \varphi_\beta}{\partial \xi^k} = 0 \quad (4.21)$$

An essential remark to be revisited is the necessity of solving the adjoint equation in reverse-time with respect to the physical or primal problem. As viewed in equation (4.18), the term (IV), related to the time conditions, must also be zero. The initial condition of the primal problem is known (imposed), therefore its virtual displacement at t_0 is zero. In other words, one remains with only an integral over the domain at t_f . It can be concluded that, in order to eliminate this term for any realizable $\delta \mathbf{Q}$, the adjoint solution must be homogeneous and equal to zero over the domain at the final instant t_f .

A convenient change of the variable t to t^* is proposed by the relation:

$$\begin{aligned} t^* &= t_f - t \\ \text{so} \\ t_0^* &= t_f \quad \text{and} \quad t_f^* = t_0 \end{aligned} \quad (4.22)$$

This leads to $dt^* = -dt$ and the adjoint equation written in the changed time basis becomes:

$$\frac{\partial \varphi_\alpha}{\partial t^*} - \frac{C_{\beta\alpha}^k}{J} \frac{\partial \varphi_\beta}{\partial \xi^k} = 0 \quad (4.23)$$

The hyperbolic characteristics of both primal and dual problems and the time-reverse relation between the equations create complementary Riemann problems when treating the boundary conditions.

4.2.1 Characteristic Form of the Adjoint Equations

The adjoint equations are similar to the Euler's equations with exception to the signal of the convective term. As an hyperbolic equation, a characteristic based description is convenient to study the appropriate boundary conditions to guarantee a well posed problem. The adjoint equation is written as:

$$\frac{\partial \varphi_\alpha}{\partial t^*} - A_{\beta\alpha} \frac{\partial \varphi_\beta}{\partial x} - B_{\beta\alpha} \frac{\partial \varphi_\beta}{\partial y} = 0 \quad (4.24)$$

The Jacobian flux matrices are transposed, and their elements $A_{\beta\alpha}$ and $B_{\beta\alpha}$. They are the components of the operator $\vec{\mathbf{A}}^T = (\mathbf{A}^T, \mathbf{B}^T)$, also represented by $A_{\beta\alpha}^i$, where

$A_{\beta\alpha}^1 = A_{\beta\alpha}$ and $A_{\beta\alpha}^2 = B_{\beta\alpha}$. The projection of the operator over a normal direction of a given boundary $\vec{k}$ is:

$$-\vec{\mathbf{A}}_K^T = -\vec{\mathbf{A}}^T \cdot \vec{k} = -k_x \mathbf{A}^T - k_y \mathbf{B}^T \quad (4.25)$$

The operator $\vec{\mathbf{A}}^T$ is a third-order tensor. The portion associated to the fluxes that cross the surface that has $\vec{k}$ as its normal vector, namely $\vec{\mathbf{A}}_K^T$, can be diagonalized and one gets:

$$-\Lambda = -\mathbf{P}^T \cdot \vec{\mathbf{A}}_K^T \cdot (\mathbf{P}^{-1})^T = \begin{bmatrix} -\mathbf{u} \cdot \mathbf{n} & 0 & 0 & 0 \\ 0 & -\mathbf{u} \cdot \mathbf{n} & 0 & 0 \\ 0 & 0 & -(\mathbf{u} \cdot \mathbf{n} + c) & 0 \\ 0 & 0 & 0 & -(\mathbf{u} \cdot \mathbf{n} - c) \end{bmatrix} \quad (4.26)$$

Due to the similarity to the Euler's equations, the diagonal terms of $\vec{\mathbf{A}}_K^T$ remain the same in absolute value but with opposite signals. The propagation of the adjoint characteristics are in opposite sense in relation to the flow ones. The matrix $\mathbf{P}^T$ associated to the $\vec{k}$ direction is:

$$\mathbf{P}^T = \begin{bmatrix} 1 & u & v & \frac{\mathbf{u} \cdot \mathbf{u}}{2} \\ 0 & \rho k_y & -\rho k_x & \rho(uk_y - vk_x) \\ \frac{\rho}{2c} & \frac{\rho(ck_x + u)}{2c} & \frac{\rho(ck_y + v)}{2c} & \frac{\rho}{2} \left(\frac{c}{\gamma - 1} + \mathbf{u} \cdot \mathbf{n} + \frac{\mathbf{u} \cdot \mathbf{u}}{2c} \right) \\ \frac{\rho}{2c} & \frac{\rho(v - ck_x)}{2c} & \frac{\rho(v - ck_y)}{2c} & \frac{\rho}{2} \left(\frac{c}{\gamma - 1} - \mathbf{u} \cdot \mathbf{n} + \frac{\mathbf{u} \cdot \mathbf{u}}{2c} \right) \end{bmatrix} \quad (4.27)$$

The characteristic form is then:

$$\underbrace{\mathbf{P}^T}_{\mathbf{K}^{t^*}} \frac{\partial \varphi}{\partial t^*} - \underbrace{\mathbf{P}^T \mathbf{A}^T (\mathbf{P}^{-1})^T}_{\mathbf{K}^{x^1=x}} \mathbf{P}^T \frac{\partial \varphi}{\partial x} - \underbrace{\mathbf{P}^T \mathbf{B}^T (\mathbf{P}^{-1})^T}_{\mathbf{K}^{x^2=y}} \mathbf{P}^T \frac{\partial \varphi}{\partial y} = 0 \quad (4.28)$$

Or

$$K_{\alpha\beta}^{t^*} \frac{\partial \varphi_\beta}{\partial t^*} = K_{\alpha\beta}^x \frac{\partial \varphi_\beta}{\partial x} + K_{\alpha\beta}^y \frac{\partial \varphi_\beta}{\partial y} \quad (4.29)$$

4.3 Adjoint Contour Problem

The adjoint boundary and time conditions are provided by terms (III) and (IV) in equation (4.18):

$$\begin{aligned}
 \text{(III)} + \text{(IV)} = & \underbrace{\left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_i}}_{\text{(III) Adjoint boundary conditions}} + \underbrace{\left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_o}}_{\text{(III) Adjoint boundary conditions}} + \\
 & \underbrace{\left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right| + \frac{\partial p}{\partial Q_\alpha} [\phi_{i'+1} J \beta_{i'}^2 n_2], \delta Q_\alpha \right\rangle_{b_w}}_{\text{(III) Adjoint boundary conditions}} + \underbrace{\left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0}^{t_f}}_{\text{(IV) Time condition}} \quad (4.30)
 \end{aligned}$$

Imposing each of the terms to be equals to zero, one find the respective conditions.

4.3.1 Time Conditions

The initial condition needed to solve the adjoint equation comes from term (IV) in equation (4.18). The key feature to work with this condition is the possibility of a reverse time variable, defined by equation (4.22).

The term (IV) is:

$$\text{(IV)} = \left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0}^{t_f} \quad (4.31)$$

The time condition is obtained when imposing (IV) to be null. Then, one needs to know the volume domain integral at t_0 and t_f . The interesting fact is that $\delta Q_\alpha|_{t_0} = 0$ once it refers to the imposed initial condition of the physical problem:

$$\begin{aligned}
 & \left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0}^{t_f} = 0 \\
 & \left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_f} - \left[\int_{\Omega} \phi_\alpha (J \delta Q_\alpha) d\Omega \right]_{t_0} \xrightarrow{0, \text{ cause } \delta Q_\alpha|_{t_0} = 0} = 0 \quad (4.32)
 \end{aligned}$$

$$\phi_\alpha|_{t_f=t_0^*} = 0 \text{ everywhere} \quad (4.33)$$

The initial condition proposed for the adjoint equation is, simply, that it be zero

everywhere. Observe, however, that one is dealing with a reverse time in relation to the physical time.

4.3.2 Boundary Conditions

From equation (4.18), one can work with terms in (III) to develop the boundary conditions. Splitting (III) in inlet, outlet and rigid wall conditions:

$$\begin{aligned}
 \text{(III)} = & \underbrace{\left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_i}}_{\text{(IIIa) Inlet condition}} + \underbrace{\left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_o}}_{\text{(IIIb) Outlet condition}} + \\
 & \underbrace{\left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right| + \frac{\partial p}{\partial Q_\alpha} [\phi_{i'+1} J \beta_{i'}^2 n_2], \delta Q_\alpha \right\rangle_{b_w}}_{\text{(IIIc) Body surface or rigid wall condition}}
 \end{aligned} \tag{4.34}$$

Equation (4.34) is a general formulation for cases in which control parameters are applied both at inlet and outlet permeable boundaries. These conditions must be analysed according to the direction in which the characteristics propagates. The next sections approach each of them for both supersonic and subsonic regimes.

4.3.2.1 Inlet

The term (IIIa) in equation (4.34) is the one to be studied to formulate the inlet boundary condition, when considering the control parameters at this permeable frontier:

$$\text{(IIIa)} = \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_i} = \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta}, \delta Q_\beta \right\rangle_{s_i} + \left\langle \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_i} \tag{4.35}$$

From the definition (2.51) of the matrix $C_{\alpha\beta}^k$ and by exchanging the variable ϕ_α for φ_α (as was done for the adjoint equations), the second term can be written in the form:

$$\left\langle \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_i} = \left\langle \varphi_\alpha A_{\alpha\beta}^{i'} n_{i'}, \delta Q_\beta \right\rangle_{s_i} \tag{4.36}$$

The objective is to cancel (IIIa). It is interesting to use the decomposition described in (1.37) to write the term in equation (4.36), since it is a bilinear concomitant:

$$\begin{aligned}
 (\text{IIIa}) &= \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta}, \delta Q_\beta \right\rangle_{s_i} + \underbrace{\left\langle \varphi_\alpha A_{\alpha\beta}^{i'} n_{i'}, \delta Q_\beta \right\rangle_{s_i}}_{\text{bilinear concomitant}} \\
 &= \langle \psi \mathbf{B}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle_{s_i} + \langle \varphi^T \mathbf{A}_k, \delta \mathbf{Q} \rangle_{s_i} \\
 &= \langle \psi \mathbf{B}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle_{s_i} + \langle P_1(\varphi), \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_{s_i} + \langle \mathbf{B}^*(\varphi), \mathbf{M} \delta \mathbf{Q} \rangle_{s_i}
 \end{aligned} \tag{4.37}$$

At this point, two cases must be analysed separately: supersonic and subsonic inlets.

Supersonic Case

At a supersonic inlet all the flow characteristics are entering the domain, meaning that one must specify all the primitive variables V_α . Evidently, the conservative variables Q_α are also defined. In other words, the control parameters would be the set of primitive variables at the inlet, however, notice that if one considers that the conditions at the boundary can vary in time according to known functions, it would be interesting to take the parameters of this function as the control parameters. In other words, these properties are given by known functions, then:

$$\text{Inlet properties} \begin{cases} \rho = f_\rho(x, y, z, t, P_\rho^k) \\ u = f_u(x, y, z, t, P_u^k) \\ v = f_v(x, y, z, t, P_v^k) \\ p = f_p(x, y, z, t, P_p^k) \end{cases} \tag{4.38}$$

Where f_i are functions of the time-space coordinates (x, y, z, t) and control parameters P^k .

What it suggests is that these properties are not defined directly, but by means of other control parameters P^k . In other words, its variations are given by:

$$\begin{aligned}
 \delta \rho &= \frac{\partial f_\rho}{\partial P_\rho^k} \delta P_\rho^k \\
 \delta u &= \frac{\partial f_u}{\partial P_u^k} \delta P_u^k \\
 \delta v &= \frac{\partial f_v}{\partial P_v^k} \delta P_v^k \\
 \delta p &= \frac{\partial f_p}{\partial P_p^k} \delta P_p^k
 \end{aligned} \tag{4.39}$$

The condition at this boundary is then:

$$\begin{aligned} \mathbf{B}[\mathbf{Q}, \mathbf{P}] = 0 &\Rightarrow \frac{\partial \mathbf{B}}{\partial \mathbf{Q}} \delta \mathbf{Q} + \frac{\partial \mathbf{B}}{\partial \mathbf{P}} \delta \mathbf{P} = 0 \\ \text{where } \frac{\partial \mathbf{B}}{\partial \mathbf{P}} \delta \mathbf{P} &= -\frac{\partial f_\alpha}{\partial P_\alpha^k} \delta P_\alpha^k \end{aligned} \quad (4.40)$$

Clearly, the variation of the inlet boundary conditions with respect to the primitive or conservative variables ($\mathbf{B}'_{\mathbf{Q}}$) is given by an identity matrix $\mathbf{I}$. Besides, as said previously, the adjoint contour conditions are complementary to the flow ones, given the minus sign of the convective term. Then, at the inlet, there is no adjoint boundary condition to be defined. In other words, the adjoint characteristics leave the domain, being part of the solution. In the absence of adjoint contour conditions $\mathbf{B}^* = 0$.

From equation (4.37), the decomposition of the bilinear concomitant can be:

$$\text{Decomposition} \quad \begin{cases} P_1(\varphi) = \varphi^T \mathbf{A}_k \\ \mathbf{B}^*(\varphi) = 0 \end{cases} \quad (4.41)$$

At the introduction of the present document, a set of implications when solving the variational problem was established. The implication number 2, given by equation (1.40), allows one to solve for ψ in terms of φ :

$$\psi = -P_1(\varphi) = -\varphi^T \mathbf{A}_k \quad (4.42)$$

Equation (4.37) can be written, according to decomposition (4.41) and (4.42), as:

$$\begin{aligned} (\text{IIIa}) &= \langle \psi \mathbf{B}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle_{s_i} + \langle P_1(\varphi), \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_{s_i} + \langle \mathbf{B}^*(\varphi), \mathbf{M} \delta \mathbf{Q} \rangle_{s_i} \\ &= \langle -\varphi^T \mathbf{A}_k \mathbf{I}, \delta \mathbf{Q} \rangle_{s_i} + \langle \varphi^T \mathbf{A}_k, \mathbf{I} \delta \mathbf{Q} \rangle_{s_i} = 0 \end{aligned} \quad (4.43)$$

The term (IIIa) is cancelled according to the requirements of the bilinear decomposition.

Subsonic Case

The subsonic inlet differs from the supersonic one with regard to the number of flow characteristics that enter and leave the domain. In this case, there are three characteristics which propagate to the interior domain and one which travels towards the outside. Consequently, it is necessary to define three inlet conditions to the flow. These can be the stagnation pressure p_0 , the stagnation temperature T_0 and the tangent of the flow

direction $\tan \theta$. To simplify the notation, the latter one is written as $\tan \theta = \vartheta$.

Again, the imposed boundary conditions given by p_0 , T_0 and ϑ are controlled by a set of parameters through generic functions as follows:

$$\text{Inlet properties} \begin{cases} p_0 = f_{p_0}(x, y, z, t, P_{p_0}^k) \\ T_0 = f_{T_0}(x, y, z, t, P_{T_0}^k) \\ \vartheta = f_{\vartheta}(x, y, z, t, P_{\vartheta}^k) \end{cases} \quad (4.44)$$

Where the control parameters are P^k . Proceeding, the variations of the imposed boundary conditions are given by:

$$\begin{aligned} \delta p_0 &= \frac{\partial f_{p_0}}{\partial P_{p_0}^k} \delta P_{p_0}^k \\ \delta T_0 &= \frac{\partial f_{T_0}}{\partial P_{T_0}^k} \delta P_{T_0}^k \\ \delta \vartheta &= \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}^k} \delta P_{\vartheta}^k \end{aligned} \quad (4.45)$$

One can write the boundary condition equations as:

$$\begin{cases} B_1(\mathbf{Q}) = p_0(\mathbf{P}) \\ B_2(\mathbf{Q}) = T_0(\mathbf{P}) \\ B_3(\mathbf{Q}) = \vartheta(\mathbf{P}) \end{cases} \quad \text{or} \quad \begin{cases} B_1(\mathbf{Q}) - p_0(\mathbf{P}) = 0 \\ B_2(\mathbf{Q}) - T_0(\mathbf{P}) = 0 \\ B_3(\mathbf{Q}) - \vartheta(\mathbf{P}) = 0 \end{cases} \quad (4.46)$$

Also, p_0 , T_0 and ϑ can be written explicitly in function of the conservative variables, with some algebra, one finds (Hayashi, 2016) [33]:

$$\begin{cases} p_0 = B_1(\mathbf{Q}) = \frac{(\gamma - 1)[2Q_1Q_4 - (Q_2^2 + Q_3^2)]}{2Q_1} \left(1 + \frac{(Q_2^2 + Q_3^2)}{\gamma[2Q_1Q_4 - (Q_2^2 + Q_3^2)]} \right)^{\frac{\gamma}{\gamma-1}} \\ T_0 = B_2(\mathbf{Q}) = \frac{(\gamma - 1)}{2\gamma R Q_1^2} [2\gamma Q_1Q_4 - (\gamma - 1)(Q_2^2 + Q_3^2)] \\ \tan(\theta) = B_3(\mathbf{Q}) = \frac{Q_3}{Q_2} \end{cases} \quad (4.47)$$

One way to calculate the variations of the state variables $\delta \mathbf{Q}$, which are used to compute the derivatives in matrices $\mathbf{B}'_{\mathbf{Q}}$ and $\mathbf{B}'_{\mathbf{P}}$, is to work with the linearized form of equation (4.46).

There is one characteristic that leaves the domain, implying that one degree of freedom must be specified, while the remaining three are left. By considering δQ_1 the free variable, one can write δQ_2 , δQ_3 and δQ_4 as functions of δQ_1 .

Equation (4.46) is linearized and δQ_1 is a free parameter:

$$\frac{\partial B_j}{\partial Q_k} \delta Q_k = \frac{\partial f_j}{\partial P_j} \delta P_j - \frac{\partial B_j}{\partial Q_1} \delta Q_1 \quad \text{with } j = 1, 2, 3 \text{ and } k = 2, 3, 4$$

or, explicitly,

$$\begin{cases} \frac{\partial B_1}{\partial Q_2} \delta Q_2 + \frac{\partial B_1}{\partial Q_3} \delta Q_3 + \frac{\partial B_1}{\partial Q_4} \delta Q_4 = \frac{\partial f_{p_0}}{\partial P_{p_0}} \delta P_{p_0} - \frac{\partial B_1}{\partial Q_1} \delta Q_1 \\ \frac{\partial B_2}{\partial Q_2} \delta Q_2 + \frac{\partial B_2}{\partial Q_3} \delta Q_3 + \frac{\partial B_2}{\partial Q_4} \delta Q_4 = \frac{\partial f_{T_0}}{\partial P_{T_0}} \delta P_{T_0} - \frac{\partial B_2}{\partial Q_1} \delta Q_1 \\ \frac{\partial B_3}{\partial Q_2} \delta Q_2 + \frac{\partial B_3}{\partial Q_3} \delta Q_3 + \frac{\partial B_3}{\partial Q_4} \delta Q_4 = \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}} \delta P_{\vartheta} - \frac{\partial B_3}{\partial Q_1} \delta Q_1 \end{cases} \quad (4.48)$$

One can solve the system of equations above in δQ_2 , δQ_3 and δQ_4 . Rearranging in the form of equation (1.30):

$$\underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial Q_1} & -1 & 0 & 0 \\ \frac{\partial Q_3}{\partial Q_1} & 0 & -1 & 0 \\ \frac{\partial Q_4}{\partial Q_1} & 0 & 0 & -1 \end{bmatrix}}_{\mathbf{B}'_{\mathbf{Q}}} \underbrace{\begin{bmatrix} \delta Q_1 \\ \delta Q_2 \\ \delta Q_3 \\ \delta Q_4 \end{bmatrix}}_{\delta \mathbf{Q}} = - \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial p_0} & \frac{\partial Q_2}{\partial T_0} & \frac{\partial Q_2}{\partial \vartheta} \\ \frac{\partial Q_3}{\partial p_0} & \frac{\partial Q_3}{\partial T_0} & \frac{\partial Q_3}{\partial \vartheta} \\ \frac{\partial Q_4}{\partial p_0} & \frac{\partial Q_4}{\partial T_0} & \frac{\partial Q_4}{\partial \vartheta} \end{bmatrix}}_{\mathbf{B}'_{\mathbf{P}}} \underbrace{\begin{bmatrix} \delta p_0 \\ \delta T_0 \\ \delta \tan(\theta) \end{bmatrix}}_{\delta \mathbf{P}} \Rightarrow$$

$$\underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial Q_1} & -1 & 0 & 0 \\ \frac{\partial Q_3}{\partial Q_1} & 0 & -1 & 0 \\ \frac{\partial Q_4}{\partial Q_1} & 0 & 0 & -1 \end{bmatrix}}_{\mathbf{B}'_{\mathbf{Q}}} \underbrace{\begin{bmatrix} \delta Q_1 \\ \delta Q_2 \\ \delta Q_3 \\ \delta Q_4 \end{bmatrix}}_{\delta \mathbf{Q}} = - \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial p_0} & \frac{\partial Q_2}{\partial T_0} & \frac{\partial Q_2}{\partial \vartheta} \\ \frac{\partial Q_3}{\partial p_0} & \frac{\partial Q_3}{\partial T_0} & \frac{\partial Q_3}{\partial \vartheta} \\ \frac{\partial Q_4}{\partial p_0} & \frac{\partial Q_4}{\partial T_0} & \frac{\partial Q_4}{\partial \vartheta} \end{bmatrix}}_{\mathbf{B}'_{\mathbf{P}}} \underbrace{\begin{bmatrix} \frac{\partial f_{p_0}}{\partial P_{p_0}} \delta P_{p_0} \\ \frac{\partial f_{T_0}}{\partial P_{T_0}} \delta P_{T_0} \\ \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}} \delta P_{\vartheta} \end{bmatrix}}_{\delta \mathbf{P}} \Rightarrow \quad (4.49)$$

$$\underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial Q_1} & -1 & 0 & 0 \\ \frac{\partial Q_3}{\partial Q_1} & 0 & -1 & 0 \\ \frac{\partial Q_4}{\partial Q_1} & 0 & 0 & -1 \end{bmatrix}}_{\mathbf{B}'_{\mathbf{Q}}} \underbrace{\begin{bmatrix} \delta Q_1 \\ \delta Q_2 \\ \delta Q_3 \\ \delta Q_4 \end{bmatrix}}_{\delta \mathbf{Q}} = - \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ \frac{\partial Q_2}{\partial p_0} \frac{\partial f_{p_0}}{\partial P_{p_0}} & \frac{\partial Q_2}{\partial T_0} \frac{\partial f_{T_0}}{\partial P_{T_0}} & \frac{\partial Q_2}{\partial \vartheta} \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}} \\ \frac{\partial Q_3}{\partial p_0} \frac{\partial f_{p_0}}{\partial P_{p_0}} & \frac{\partial Q_3}{\partial T_0} \frac{\partial f_{T_0}}{\partial P_{T_0}} & \frac{\partial Q_3}{\partial \vartheta} \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}} \\ \frac{\partial Q_4}{\partial p_0} \frac{\partial f_{p_0}}{\partial P_{p_0}} & \frac{\partial Q_4}{\partial T_0} \frac{\partial f_{T_0}}{\partial P_{T_0}} & \frac{\partial Q_4}{\partial \vartheta} \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}} \end{bmatrix}}_{\mathbf{B}'_{\mathbf{P}}} \underbrace{\begin{bmatrix} \delta P_{p_0} \\ \delta P_{T_0} \\ \delta P_{\vartheta} \end{bmatrix}}_{\delta \mathbf{P}}$$

On computing matrices $\mathbf{B}'_{\mathbf{Q}}$ and $\mathbf{B}'_{\mathbf{P}}$:

$$\mathbf{B}'_{\mathbf{Q}} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ u - \frac{\gamma pu}{\rho(u^2+v^2)} & -1 & 0 & 0 \\ v - \frac{\gamma pv}{\rho(u^2+v^2)} & 0 & -1 & 0 \\ \frac{-\rho u^2 + \gamma[-2(-2+\gamma)p + \rho u^2] + (\gamma-1)\rho v^2}{2(\gamma-1)\rho} & 0 & 0 & -1 \end{bmatrix} \quad (4.50)$$

$$\mathbf{B}'_{\mathbf{P}} = \begin{bmatrix} 0 & 0 & 0 \\ \frac{\rho u}{M^2 p_0} \frac{\partial f_{p_0}}{\partial P_{p_0}} & \frac{u}{2T_0} \left(\rho - \frac{2\rho}{M^2} \right) \frac{\partial f_{T_0}}{\partial P_{T_0}} & \frac{\rho^2 u^2 v}{\gamma M^2} p \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}} \\ \frac{\rho v}{M^2 p_0} \frac{\partial f_{p_0}}{\partial P_{p_0}} & \frac{v}{2T_0} \left(\rho - \frac{2\rho}{M^2} \right) \frac{\partial f_{T_0}}{\partial P_{T_0}} & \frac{\rho^2 u^3}{\gamma M^2} p \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}} \\ \frac{(\gamma-1)p}{p_0} \frac{\partial f_{p_0}}{\partial P_{p_0}} & \frac{\gamma p}{T} \left(\frac{1}{\gamma-1} - \frac{T}{T_0} \right) \frac{\partial f_{T_0}}{\partial P_{T_0}} & 0 \end{bmatrix} \quad (4.51)$$

An important remark is that the operator $\mathbf{B}'_{\mathbf{Q}}$ presented in this work, which was computed by Hayashi (2016) [33], is equivalent to equation (43) from Hayashi, Ceze and Volpe (2013) [31]. According to Hayashi (2016) [33], this allows the use of the same adjoint boundary condition used in their previous work. This assertion is specially interesting, since the boundary conditions from Hayashi, Ceze and Volpe (2013) [31] were derived without considering the control parameters δP related to the properties at the boundaries, differently from the present approach, which is based on the general formulation by Cacuci (1980) [2]. The technical report made by Volpe (2013) [36] discusses this assertion in details for the unsteady Navier-Stokes incompressible flow, which indicates that the same adjoint boundary condition for the approach based only in geometry variations can be used for the general case.

Actually, this is one of the main features of the approach by Cacuci (1980) [2], because it extends the traditional formulation used for geometric sensitivities (related to the geometry of the domain) to non-geometric sensitivities (related to properties at the permeable boundaries) without greater changes in the adjoint boundary conditions.

That being said, the adjoint condition used by Hayashi, Ceze and Volpe (2013) [31] is:

$$C_1 \varphi_1 + C_2 \varphi_2 + C_3 \varphi_3 + C_4 \varphi_4 = 0 \quad (4.52)$$

Where:

$$\begin{cases}
 C_1 = \left[2 - \gamma + \gamma^2 - \frac{2\gamma e (\gamma - 1)}{u^2 + v^2} \right] \frac{(k_x u + k_y v)}{2} \\
 C_2 = \frac{(2 - \gamma + \gamma^2) k_x u^2 + 2(1 - \gamma + \gamma^2) k_y uv}{2} - \frac{(\gamma - 1) \gamma k_x v^2}{2} \\
 \quad - \frac{2\gamma e (\gamma - 1) [2k_y uv + k_x (u^2 - v^2)]}{2(u^2 + v^2)} \\
 C_3 = \frac{-\gamma (\gamma - 1) k_y u^4 + 2k_y u^2 v^2}{2(u^2 + v^2)} \\
 \quad + \frac{2(1 - \gamma + \gamma^2) (u^3 v + uv^3) k_x + (2 - \gamma + \gamma^2) k_y v^4 + 2\gamma e (\gamma - 1) [k_y (u^2 - v^2) - 2k_x uv]}{2(u^2 + v^2)} \\
 C_4 = -\frac{(k_x u + k_y v) [(\gamma - 1) (u^2 + v^2) - 2\gamma e] [(2 - \gamma + \gamma^2) (u^2 + v^2) - 2\gamma e (\gamma - 1)]}{4(u^2 + v^2)}
 \end{cases} \quad (4.53)$$

Analogous to what was done for the supersonic case, one can decompose the bilinear concomitant from equation (4.37). However, on considering that in the subsonic case there is one adjoint characteristic entering the domain, the adjoint boundary operator $\mathbf{B}^*$ is non zero. The decomposition becomes:

$$\text{Decomposition} \quad \begin{cases} P_1(\varphi) = -\varphi^T \mathbf{A}_k \\ \mathbf{B}^*(\varphi) = \varphi^T \mathbf{B}^{*T} \end{cases} \quad (4.54)$$

And the adjoint boundary operator $\mathbf{B}^*$ refers to the equation (4.52):

$$\mathbf{B}^* = \begin{bmatrix} 1 & -\frac{C_2}{C_1} & -\frac{C_3}{C_1} & -\frac{C_4}{C_1} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.55)$$

From equation (4.37), ψ and $\mathbf{M}$ remain as yet undetermined. The term $\mathbf{M}$ is obtained simply by making:

$$\mathbf{M} = \sqrt{g_{11}} \begin{bmatrix} M_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{with} \quad M_{11} = (2 - \gamma + \gamma^2) (k_x + k_y) - \frac{\gamma e (\gamma - 1)}{u^2 + v^2} (k_x u + k_y v) \quad (4.56)$$

On observing that $\sqrt{g_{11}}$ is the component of the metric tensor related to the generalized coordinates change.

The term ψ is, again by (1.40), solved for:

$$\psi = -P_1(\varphi) = \varphi^T \mathbf{A}_k \quad (4.57)$$

With the conclusion established, equation (4.37) for the term (IIIa) becomes:

$$\begin{aligned} \text{(IIIa)} &= \langle \psi \mathbf{B}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle_{s_i} + \langle P_1(\varphi), \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_{s_i} + \langle \mathbf{B}^*(\varphi), \mathbf{M} \delta \mathbf{Q} \rangle_{s_i} \\ &= \langle \varphi^T \mathbf{A}_k \mathbf{I}, \delta \mathbf{Q} \rangle_{s_i} - \langle \varphi^T \mathbf{A}_k, \mathbf{I} \delta \mathbf{Q} \rangle_{s_i} + \langle \mathbf{B}^*(\varphi), \mathbf{M} \delta \mathbf{Q} \rangle_{s_i} = 0 \end{aligned} \quad (4.58)$$

The term (IIIa) is null as expected.

4.3.2.2 Outlet

The adjoint condition at the outlet comes from the term (IIIb) in equation (4.34). Clearly, the terms (IIIa) and (IIIb) are similar, but computed at the inlet and outlet, respectively. Thus, the same approach can be used. (IIIb) is:

$$\text{(IIIb)} = \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta} + \phi_\alpha C_{\alpha\beta}^k n_k, \delta Q_\beta \right\rangle_{s_o} \quad (4.59)$$

Which can be written as:

$$\begin{aligned} \text{(IIIb)} &= \left\langle \psi_\alpha \frac{\partial B_\alpha}{\partial Q_\beta}, \delta Q_\beta \right\rangle_{s_o} + \underbrace{\left\langle \varphi_\alpha A_{\alpha\beta}^{i'} n_{i'}, \delta Q_\beta \right\rangle_{s_o}}_{\text{bilinear concomitant}} \\ &= \langle \psi \mathbf{B}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle_{s_o} + \langle \varphi^T \mathbf{A}_k, \delta \mathbf{Q} \rangle_{s_o} \\ &= \langle \psi \mathbf{B}'_{\mathbf{Q}}, \delta \mathbf{Q} \rangle_{s_o} + \langle P_1(\varphi), \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_{s_o} + \langle \mathbf{B}^*(\varphi), \mathbf{M} \delta \mathbf{Q} \rangle_{s_o} \end{aligned} \quad (4.60)$$

Again, one shall impose that equation (4.60) be null. As the propagation sense of the characteristics relies on the flow regime (subsonic or supersonic), the outlet conditions are treated in separate cases.

Supersonic Case

For the supersonic outlet it is interesting to remember that no physical conditions are imposed. Hence any variation $\delta \mathbf{Q}$ is possible. The adjoint condition to be imposed is

then suggested by Hayashi (2016) [33] to be homogeneous:

$$\varphi_i|_{s_o} = 0 \quad (4.61)$$

Subsonic Case

The subsonic case for the outlet is treated similarly as the subsonic inlet. Notice that there is only one physical condition imposed: the static pressure p . Hence, the adjoint counterpart requires three boundary conditions, while the fourth is determined by the interior domain.

Again, the outlet static pressure can be given by some function which is controlled by the parameters P^k :

$$\text{Outlet property } \left\{ p = f_p(x, y, z, t, P_p^k) \right. \quad (4.62)$$

While its variation is:

$$\delta p = \frac{\partial f_p}{\partial P_p^k} \delta P_p^k \quad (4.63)$$

The equation for the physical boundary can be written:

$$\mathbf{B}[\mathbf{Q}] = p(\mathbf{P}) \Rightarrow B_4(\mathbf{Q}) = p(\mathbf{P}) \quad \text{or} \quad \mathbf{B}[\mathbf{Q}, \mathbf{P}] = 0 \Rightarrow B_4(\mathbf{Q}) - p(\mathbf{P}) = 0 \quad (4.64)$$

The relation of p with the conservative variables is presented as:

$$p = B_4(\mathbf{Q}) = (\gamma - 1) \left(Q_4 - \frac{Q_2^2 + Q_3^2}{2Q_1} \right) \quad (4.65)$$

In order to compute $\mathbf{B}'_{\mathbf{Q}}$ and $\mathbf{B}'_{\mathbf{P}}$, again it is useful to take the linearized form of equation (4.64) and to write it as (4.40). Thus one gets:

$$\begin{aligned} \frac{\partial B_4}{\partial Q_k} \delta Q_k &= \frac{\partial f_p}{\partial P_p} \delta P_p \quad \text{with } k = 1, 2, 3, 4 \\ \Rightarrow \frac{\partial B_4}{\partial Q_4} \delta Q_4 &= \frac{\partial f_p}{\partial P_p} \delta P_p - \frac{\partial B_4}{\partial Q_1} \delta Q_1 - \frac{\partial B_4}{\partial Q_2} \delta Q_2 - \frac{\partial B_4}{\partial Q_3} \delta Q_3 \end{aligned} \quad (4.66)$$

And due to (4.65) one obtains:

$$\delta Q_4 = \frac{1}{(\gamma - 1)} \frac{\partial f_p}{\partial P_p} \delta P_p - \frac{(u^2 + v^2)}{2} \delta Q_1 + u \delta Q_2 + v \delta Q_3 \quad (4.67)$$

Which can be cast in operator form as:

$$\underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{(u^2+v^2)}{2} & -u & -v & 1 \end{bmatrix}}_{\mathbf{B}'_{\mathbf{Q}}} \underbrace{\begin{bmatrix} \delta Q_1 \\ \delta Q_2 \\ \delta Q_3 \\ \delta Q_4 \end{bmatrix}}_{\delta \mathbf{Q}} = - \underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{1}{\gamma-1} \frac{\partial f_p}{\partial P_p} \end{bmatrix}}_{\mathbf{B}'_{\mathbf{P}}} \underbrace{\begin{bmatrix} \delta P_p \end{bmatrix}}_{\delta \mathbf{P}} \quad (4.68)$$

Again, it is highlighted the similarity between $\mathbf{B}'_{\mathbf{Q}}$ found above and the one derived by Hayashi (2016) [33]. Although the latter did not consider a controlled outlet, the observation made in the subsonic inlet development indicates that one could use the same adjoint boundary condition from that work. In fact, it would be an analogous consideration to the assumption made by Hayashi (2016) [33] with respect to the work from Hayashi, Ceze and Volpe (2013) [31] for the subsonic inlet or the remark made by Volpe (2013) [36]. It implies that the same adjoint boundary condition derived for the geometric case can be used for the non-geometric one:

$$\begin{cases} \varphi_1 - C_1 \varphi_4 = 0 \\ \varphi_2 - C_2 \varphi_4 = 0 \\ \varphi_3 - C_3 \varphi_4 = 0 \end{cases} \quad (4.69)$$

Where the coefficients C are given by:

$$\begin{cases} C_1 = \frac{1}{2} [2e_t \gamma - (\gamma - 1) (u^2 + v^2)] \varphi_4 \\ C_2 = \left[\frac{-2e_t \gamma k_x + (\gamma - 2) k_x u^2 - 2k_y uv + \gamma k_x v^2}{2 (k_x u + k_y v)} \right] \varphi_4 \\ C_3 = \left[\frac{-2e_t \gamma k_y + (\gamma - 2) k_y v^2 - 2k_x uv + \gamma k_y u^2}{2 (k_x u + k_y v)} \right] \varphi_4 \end{cases} \quad (4.70)$$

Which can also be cast in operator form, as follows:

$$\mathbf{B}^* = \begin{bmatrix} 1 & 0 & 0 & -C_1 \\ 0 & 1 & 0 & -C_2 \\ 0 & 0 & 1 & -C_3 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.71)$$

And the decomposition of the bilinear concomitant can be:

$$\text{Decomposition} \quad \begin{cases} P_1(\varphi) = -\varphi^T \mathbf{A}_k \\ \mathbf{B}^*(\varphi) = \varphi^T \mathbf{B}^{*T} \end{cases} \quad (4.72)$$

To find $\mathbf{M}$ it suffices to write explicitly the bilinear concomitant decomposition:

$$\begin{aligned} \langle \varphi^T \cdot \mathbf{A}_k, \delta \mathbf{Q} \rangle_{s_o} &= \langle P_1(\varphi), \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_{s_o} + \langle \mathbf{B}^*(\varphi), \mathbf{M} \delta \mathbf{Q} \rangle_{s_o} = \\ &= -\langle \varphi^T \mathbf{A}_k, \mathbf{B}'_{\mathbf{Q}} \delta \mathbf{Q} \rangle_{s_o} + \langle \varphi^T \mathbf{B}^{*T}, \mathbf{M} \delta \mathbf{Q} \rangle_{s_o} \end{aligned} \quad (4.73)$$

And:

$$\langle \varphi^T \cdot \mathbf{A}_k, (\mathbf{I} + \mathbf{B}'_{\mathbf{Q}}) \delta \mathbf{Q} \rangle_{s_o} = \langle \varphi^T \mathbf{B}^{*T}, \mathbf{M} \delta \mathbf{Q} \rangle_{s_o} \quad (4.74)$$

The operator $\mathbf{M}$ at the outlet is then:

$$\mathbf{M} = \sqrt{g_{11}} \begin{bmatrix} 0 & k_x & k_y & 0 \\ -u(\mathbf{u} \cdot \mathbf{n}) & k_x u + \mathbf{u} \cdot \mathbf{n} & k_y u & 0 \\ -v(\mathbf{u} \cdot \mathbf{n}) & k_x v & k_y v + \mathbf{u} \cdot \mathbf{n} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (4.75)$$

4.3.2.3 Solid Wall

The condition at the solid walls is determined by the term (IIIc):

$$(\text{IIIc}) = \left\langle \frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right| + \frac{\partial p}{\partial Q_\alpha} [\phi_{i'+1} J \beta_{i'}^2 n_2], \delta Q_\alpha \right\rangle_{b_w} \quad (4.76)$$

And one shall impose (IIIc) to be zero for any realizable δQ_α , conducting to:

$$\frac{\partial \mathcal{F}}{\partial Q_\alpha} \left| \frac{dS'}{dS} \right| = -\frac{\partial p}{\partial Q_\alpha} [\phi_{i'+1} J \beta_{i'}^2 n_2] \quad \text{at the solid wall} \quad (4.77)$$

Observing that the ratio between the area elements in the original and transformed coordinates is $\sqrt{g_{11}}$, element of the metric tensor, and $\phi_{i'+1} J \beta_{i'}^2 n_2 = \phi_{i'+1} n_{i'}|_{b_w}$, the wall condition is simply:

$$k_x \varphi_2 + k_y \varphi_3 = \frac{\partial \mathcal{F}}{\partial p} \sqrt{g_{11}} \quad (4.78)$$

4.4 Gradient

The gradient comes from term (V), rewritten as follows:

$$\begin{aligned} (V) = & \left[\left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_i} + \left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_o} \right]_{=\text{farfield}} + \left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle_{b_w} + \\ & \left\langle \phi_\alpha, \frac{\partial (Q_\alpha \delta J)}{\partial t} \right\rangle - \left\langle \delta (J \beta_{i'}^k), \frac{f_\alpha^{i'}}{J} \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \right\rangle + \langle p, [\phi_{i'+1} \delta (J \beta_{i'}^2) n_2] \rangle_{b_w} + \\ & \langle \psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s + \langle \mathbf{a}, \delta \mathbf{P} \rangle \end{aligned} \quad (4.79)$$

And the gradient is computed as:

$$\begin{aligned} \langle \mathbf{a}, \delta \mathbf{P} \rangle = & - \left[\left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_i} + \left\langle \phi_\alpha, \delta (J \beta_{i'}^k) f_\alpha^{i'} n_k \right\rangle_{s_o} \right]_{=\text{farfield}} - \left\langle \mathcal{F}, \delta \left| \frac{dS'}{dS} \right| \right\rangle_{b_w} + \\ & - \left\langle \phi_\alpha, \frac{\partial (Q_\alpha \delta J)}{\partial t} \right\rangle + \left\langle \delta (J \beta_{i'}^k), \frac{f_\alpha^{i'}}{J} \frac{\partial (J \phi_\alpha)}{\partial \xi^k} \right\rangle - \langle p, [\phi_{i'+1} \delta (J \beta_{i'}^2) n_2] \rangle_{b_w} + \\ & - \langle \psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s \end{aligned} \quad (4.80)$$

However, if no geometrical variation is considered, the gradient can be computed only by:

$$\langle \mathbf{a}, \delta \mathbf{P} \rangle = - \langle \psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_s \quad (4.81)$$

The remaining term is then related to the inlet and outlet sensitivities. If one aims to compute the sensitivity with respect to an inlet control parameter, the surface integral can be restricted to the corresponding boundary, on the other hand, if the objective is to calculate the derivative with respect to an outlet parameter, then the integral should be evaluated at the outlet surface.

$$\langle \mathbf{a}, \delta \mathbf{P} \rangle = \begin{cases} -\langle \psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_{s_i} & (\text{sensitivity with respect to an inflow parameter}) \\ -\langle \psi, \mathbf{B}'_{\mathbf{P}} \delta \mathbf{P} \rangle_{s_o} & (\text{sensitivity with respect to an outflow parameter}) \end{cases} \quad (4.82)$$

The gradient is computed with respect to the P_{α}^k for a controlled inlet and supersonic flow with equation (4.83).

$$\begin{cases} \frac{\partial I}{\partial P_{\rho}^k} = \int_{t_o}^{t_f} \int_{s_i} \left(-U_n \varphi_1 - u U_n \varphi_2 - v U_n \varphi_3 - \frac{1}{2} c^2 U_n M^2 \varphi_4 \right) \frac{\partial f_{\rho}}{\partial P_{\rho}^k} dS dt \\ \frac{\partial I}{\partial P_u^k} = \int_{t_o}^{t_f} \int_{s_i} [-k_x \rho \varphi_1 - \rho (k_x u + U_n) \varphi_2 - \rho v k_x \varphi_3 + (-k_x \sigma - \rho u U_n) \varphi_4] \frac{\partial f_u}{\partial P_u^k} dS dt \\ \frac{\partial I}{\partial P_v^k} = \int_{t_o}^{t_f} \int_{s_i} [-k_y \rho \varphi_1 - \rho u k_y \varphi_2 - \rho (k_y v + U_n) \varphi_3 + (-k_y \sigma - \rho u U_n) \varphi_4] \frac{\partial f_v}{\partial P_v^k} dS dt \\ \frac{\partial I}{\partial P_p^k} = \int_{t_o}^{t_f} \int_{s_i} \left(-k_x \varphi_2 - k_y \varphi_3 - \frac{\gamma U_n}{\gamma - 1} \varphi_4 \right) \frac{\partial f_p}{\partial P_p^k} dS dt \end{cases} \quad (4.83)$$

And for the subsonic case, the sensitivities at the inlet are computed by equations (4.84) and at the outlet by equation (4.85).

$$\begin{cases} \frac{\partial I}{\partial P_{p_0}^k} = \int_{t_o}^{t_f} \int_{s_i} \left[\left(\frac{\rho U_n}{p_0 M^2} \right) \varphi_1 + \left(\frac{(1 - \gamma) k_x p M^2 + 2 \rho u U_n}{p_0 M^2} \right) \varphi_2 + \right. \\ \left. \left(\frac{(1 - \gamma) k_y p M^2 + 2 \rho v U_n}{p_0 M^2} \right) \varphi_3 + \left(\frac{[2 + (\gamma - 1) M^2] \gamma p U_n}{2 (\gamma - 1) p_0 M^2} \right) \varphi_4 \right] \frac{\partial f_{p_0}}{\partial P_{p_0}^k} dS dt \\ \frac{\partial I}{\partial P_{T_0}^k} = \int_{t_o}^{t_f} \int_{s_i} \left[\left(\frac{(M^2 - 2) \rho U_n}{2 T_0 M^2} \right) \varphi_1 + \left(\frac{(M^2 - 2) \rho u U_n + \gamma p k_x M^2}{T_0 M^2} \right) \varphi_2 + \right. \\ \left. \left(\frac{(M^2 - 2) \rho v U_n + \gamma p k_y M^2}{T_0 M^2} \right) \varphi_3 + \left(\frac{(3 M^2 - 2) \gamma p U_n}{2 (\gamma - 1) T M^2} \right) \varphi_4 \right] \frac{\partial f_{T_0}}{\partial P_{T_0}^k} dS dt \\ \frac{\partial I}{\partial P_{\vartheta}^k} = \int_{t_o}^{t_f} \int_{s_i} \left[\left(\frac{(k_y u - k_x v) \rho u^2}{u^2 + v^2} \right) \varphi_1 + \left(\frac{k_y (u^2 - v^2) - 2 k_x u v}{u^2 + v^2} \rho u^2 \right) \varphi_2 + \right. \\ \left. \left(\frac{k_x (u^2 - v^2) - 2 k_y u v}{u^2 + v^2} \rho u^2 \right) \varphi_3 + \left((k_y u - k_x v) \rho u^2 \left(\frac{1}{2} + \frac{1}{(\gamma - 1) M^2} \right) \right) \varphi_4 \right] \frac{\partial f_{\vartheta}}{\partial P_{\vartheta}^k} dS dt \end{cases} \quad (4.84)$$

$$\frac{\partial I}{\partial P_p^k} = \int_{t_o}^{t_f} \int_{s_o} \left[-k_x \varphi_2 - k_y \varphi_3 - \frac{\gamma U_n}{\gamma - 1} \varphi_4 \right] \frac{\partial f_p}{\partial P_p^k} dS dt \quad (4.85)$$

The gradient is computed after solving both physical and adjoint problems with the help of equations (4.84), (4.83) and (4.85).

For each correspondent time step t and t^* , the surface integral is computed and then, the integration over time is made with a trapezoidal method.

5 NUMERICAL METHOD: ADJOINT PROBLEM

The numerical approach to solve the adjoint equations is similar to the one used by Hayashi (2016) [33]. Notice, however, that the time-dependent adjoint problem requires the complete time-history of the physical problem. The chapter has the objective to show the numerical method that was implemented in the code, in a way that emphasizes the precautions one must take to obtain an accurate transient solution.

5.1 Spatial Discretization

The code itself has a similar structure to solve both physical and adjoint equations. However, some considerations must be made. Despite the similarity between the Euler's Equations and the adjoint ones, they were formulated in slightly different ways.

The adjoint equation is written:

$$\frac{\partial \Psi}{\partial t^*} - \mathbf{A}^T \frac{\partial \Psi}{\partial x} - \mathbf{B}^T \frac{\partial \Psi}{\partial y} = 0 \quad (5.1)$$

with $\mathbf{A} = \mathbf{A}(t^*)$ and $\mathbf{B} = \mathbf{B}(t^*)$

As it can be seen, the adjoint equation is written in a reverse time t^* dependency. The solution method is based on computing the spatial derivatives as equations (5.2):

$$\begin{aligned} \left(\frac{\partial f}{\partial x} \right)_i &\approx \frac{1}{2\Omega_i} \sum_k (f_i + f_k) \Delta x_{ik} \\ \left(\frac{\partial f}{\partial y} \right)_i &\approx \frac{1}{2\Omega_i} \sum_k (f_i + f_k) \Delta y_{ik} \end{aligned} \quad (5.2)$$

Where f can be a general function. So, in terms of Ψ :

$$\begin{aligned}
\left(\frac{\partial \Psi}{\partial x}\right)_i &\approx \frac{1}{\Omega_i} \sum_k \Psi_{ik} \Delta x_{ik} \\
\left(\frac{\partial \Psi}{\partial y}\right)_i &\approx \frac{1}{\Omega_i} \sum_k \Psi_{ik} \Delta y_{ik} \\
\text{where } \Psi_{ik} &= \frac{1}{2} (\Psi_i + \Psi_k)
\end{aligned} \tag{5.3}$$

The derivatives are, then, multiplied by the matrices $\mathbf{A}^T$ and $\mathbf{B}^T$. It is important to mention that both matrices are time-dependent, so they must be updated at each time step. As their inputs are functions of the flow variables, the information of the physical solution at each time is required. Nevertheless, the adjoint solution runs in a reverse time, which implies that the information from the physical problem has to be read reversely.

Figure 2: Correspondence between t and t^*

The convective term is then:

$$C(\Psi) = \mathbf{A}_i^T(t^*) \left[\frac{1}{\Omega_i} \sum_k \Psi_{ik} \Delta y_{ik} \right] - \mathbf{B}_i^T(t^*) \left[\frac{1}{\Omega_i} \sum_k \Psi_{ik} \Delta x_{ik} \right] \tag{5.4}$$

And the semi-discretized adjoint equation is written as:

$$\frac{\partial \Psi}{\partial t^*} - C(\Psi) = 0 \tag{5.5}$$

However, as it happens with the Euler Equations, an artificial dissipative term $D(\Psi)$ must be implemented, however with opposite signal:

$$\frac{\partial (\Psi_i \Omega_i)}{\partial t^*} - C(\Psi) - D(\Psi) = 0 \quad \text{with} \quad \Psi_i = \frac{1}{\Omega_i} \int_{\Omega_i} \Psi dx dy \tag{5.6}$$

Where $D(\Psi)$ is defined analogously as $D(\mathbf{Q})$.

5.2 Time Integration

The semi-discretized equation (5.6) is now a ODE with respect to time:

$$\frac{d\Psi_i}{dt^*} = \frac{1}{\Omega_i} [C(\Psi) + D(\Psi)] \quad (5.7)$$

The time integration is made by a Runge-Kutta of 5 steps and second-order precision:

$$\begin{aligned} \Psi_i^{(0)} &= \Psi_i^{(n)} \\ \Psi_i^{(1)} &= \Psi_i^{(0)} + \alpha_1 \frac{\Delta t^*}{\Omega_i} [C(\Psi_i^{(0)}) + D(\Psi_i^{(0)})] \\ \Psi_i^{(2)} &= \Psi_i^{(0)} + \alpha_2 \frac{\Delta t^*}{\Omega_i} [C(\Psi_i^{(1)}) + D(\Psi_i^{(1)})] \\ \Psi_i^{(3)} &= \Psi_i^{(0)} + \alpha_3 \frac{\Delta t^*}{\Omega_i} [C(\Psi_i^{(2)}) + D(\Psi_i^{(1)})] \\ \Psi_i^{(4)} &= \Psi_i^{(0)} + \alpha_4 \frac{\Delta t^*}{\Omega_i} [C(\Psi_i^{(3)}) + D(\Psi_i^{(1)})] \\ \Psi_i^{(5)} &= \Psi_i^{(0)} + \alpha_5 \frac{\Delta t^*}{\Omega_i} [C(\Psi_i^{(4)}) + D(\Psi_i^{(1)})] \\ \Psi_i^{(n+1)} &= \Psi_i^{(5)} \end{aligned} \quad (5.8)$$

Where the α_i 's are:

$$\alpha_1 = \frac{1}{4}, \alpha_2 = \frac{1}{6}, \alpha_3 = \frac{3}{8}, \alpha_4 = \frac{1}{2} \text{ and } \alpha_5 = 1 \quad (5.9)$$

5.3 Boundary Conditions

The boundary conditions are treated using the characteristic method as it was done with the Euler's Equations. However, other important aspects are highlighted throughout the development made in this section.

As said previously, the similarity between the physical and adjoint equations permits that, given a well-posed physical problem, to define an equally well-posed adjoint problem. The minus signal in the convective term of the adjoint equations, which is the only mathematical operation that differs from its counterpart in the Euler equations, implies a reversal in the characteristics direction, as compared to the latter. This is represented

by the diagonalized matrix (4.26) from the adjoint equation:

$$-\Lambda = -\mathbf{P}^T \cdot \vec{\mathbf{A}}_K^T \cdot (\mathbf{P}^{-1})^T = \begin{bmatrix} -\mathbf{u} \cdot \mathbf{n} & 0 & 0 & 0 \\ 0 & -\mathbf{u} \cdot \mathbf{n} & 0 & 0 \\ 0 & 0 & -(\mathbf{u} \cdot \mathbf{n} + c) & 0 \\ 0 & 0 & 0 & -(\mathbf{u} \cdot \mathbf{n} - c) \end{bmatrix} \quad (5.10)$$

According to the number of characteristics entering or leaving the domain, it is possible to decide how many imposed adjoint conditions are needed (the ones found in the previous chapter) and the compatibility relations to make the adjoint problem well-posed..

5.3.1 Inlet

At the inlet, three of the diagonal terms are always negative: $-\mathbf{u} \cdot \mathbf{n}$ (multiplicity 2) and $-(\mathbf{u} \cdot \mathbf{n} + c)$. At this type of boundary, $\mathbf{u}$ and $\mathbf{n}$ have the same direction and signal. However, $-(\mathbf{u} \cdot \mathbf{n} - c)$ is negative when the flow is supersonic and positive otherwise. Notice that it is exactly the opposite from the Euler's Equations.

5.3.1.1 Supersonic Case

With all four terms in (4.26) being negative, all their associated characteristics leave the domain. This implies in no imposed adjoint conditions at the supersonic inlet. Therefore, all the information to define the state of the ghost cell comes from the compatibility relations, as represented on table 5.

It is sufficient to solve the linear system on table 5 in $\frac{\partial \varphi_i}{\partial t^\star}$ and the evolution of the adjoint variables at the ghost cells are defined:

$$\varphi_{i,ghost}^{n+1} = \varphi_{i,ghost}^n + \frac{\partial \varphi_i}{\partial t^\star} \Delta t^\star \quad (5.11)$$

5.3.1.2 Subsonic Case

A subsonic inlet implies in $-(\mathbf{u} \cdot \mathbf{n} - c) > 0$, thus, the associated characteristic enters the domain. It requires that an adjoint boundary condition be imposed. This condition comes from equation (4.52), from the development of term (IIIa) in equation (4.34). The table 6 shows the information discussed.

Table 5: Adjoint conditions and compatibility relations at the supersonic inlet

Characteristics entering the domain	0
Characteristics leaving the domain	4
Imposed adjoint conditions	-
Numerical conditions/Compatibility relations	$K_{11}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{12}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{13}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{14}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_1$ $K_{21}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{22}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{23}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{24}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_2$ $K_{31}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{32}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{33}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{34}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_3$ $K_{41}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{42}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{43}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{44}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_4$

Table 6: Adjoint conditions and compatibility relations at the subsonic inlet

Characteristics entering the domain	1
Characteristics leaving the domain	3
Imposed adjoint conditions	$C_1 \varphi_1 + C_2 \varphi_2 + C_3 \varphi_3 + C_4 \varphi_4 = 0$
Numerical conditions/Compatibility relations	$K_{11}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{12}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{13}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{14}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_1$ $K_{21}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{22}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{23}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{24}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_2$ $K_{31}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{32}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{33}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{34}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_3$

To update a ghost cell properly, the evolution of all its information ($\delta \varphi_i$) must come from the equations in table 6. This can be achieved via two different forms: by solving the equations as they appear; or by deriving equation (4.52) and by solving the set in $\frac{\partial \varphi}{\partial t^*}$. From the point of view of numerical methods, the latter seems to be far more practical. The system to be solved is then:

$$\begin{cases} K_{11}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{12}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{13}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{14}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_1 \\ K_{21}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{22}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{23}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{24}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_2 \\ K_{31}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{32}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{33}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{34}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_3 \\ C_1 \frac{\partial \varphi_1}{\partial t^*} + \frac{\partial C_1}{\partial t^*} \varphi_1 + C_2 \frac{\partial \varphi_2}{\partial t^*} + \frac{\partial C_2}{\partial t^*} \varphi_2 + C_3 \frac{\partial \varphi_3}{\partial t^*} + \frac{\partial C_3}{\partial t^*} \varphi_3 + C_4 \frac{\partial \varphi_4}{\partial t^*} + \frac{\partial C_4}{\partial t^*} \varphi_4 = 0 \end{cases} \quad (5.12)$$

The fact that one is dealing with a time-dependent problem, in which boundary conditions are not constant in time, implies the necessity of computing the terms $\frac{\partial C_i}{\partial t^*}$. To do so, the following simple finite difference approximation is assumed:

$$\frac{\partial C_i}{\partial t^*} \approx \frac{C_i(t^* + \Delta t^*) - C_i(t^* - \Delta t^*)}{2\Delta t^*} \quad (5.13)$$

And the $C_i(t^*)$ are taken from the physical solution at the corresponding physical t . The work made by Hayashi (2016) [33] focuses in steady-state flows and, thus, $\frac{\partial C_i}{\partial t^*} = 0$, so only the steady-state physical solution is needed to solve the adjoint problem.

The system becomes:

$$\begin{cases} K_{11}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{12}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{13}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{14}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_1 \\ K_{21}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{22}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{23}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{24}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_2 \\ K_{31}^{t^*} \frac{\partial \varphi_1}{\partial t^*} + K_{32}^{t^*} \frac{\partial \varphi_2}{\partial t^*} + K_{33}^{t^*} \frac{\partial \varphi_3}{\partial t^*} + K_{34}^{t^*} \frac{\partial \varphi_4}{\partial t^*} = R_3 \\ C_1 \frac{\partial \varphi_1}{\partial t^*} + C_2 \frac{\partial \varphi_2}{\partial t^*} + C_3 \frac{\partial \varphi_3}{\partial t^*} + C_4 \frac{\partial \varphi_4}{\partial t^*} = - \left[\frac{C_1(t^* + \Delta t^*) - C_1(t^* - \Delta t^*)}{2\Delta t^*} \right] \varphi_1(t^*) + \\ - \left[\frac{C_2(t^* + \Delta t^*) - C_2(t^* - \Delta t^*)}{2\Delta t^*} \right] \varphi_2(t^*) - \left[\frac{C_3(t^* + \Delta t^*) - C_3(t^* - \Delta t^*)}{2\Delta t^*} \right] \varphi_3(t^*) + \\ - \left[\frac{C_4(t^* + \Delta t^*) - C_4(t^* - \Delta t^*)}{2\Delta t^*} \right] \varphi_4(t^*) \end{cases} \quad (5.14)$$

The φ_i are taken at time t^* . With the solution of the system, one can compute the evolution of the ghost cells:

$$\varphi_{i,ghost}^{n+1} = \varphi_{i,ghost}^n + \frac{\partial \varphi_i}{\partial t^*} \Delta t \quad (5.15)$$

5.3.2 Outlet

The outlet has three characteristics that always enter the domain and one whose sense depends to the flow regime. The same methodology from the inlet boundary conditions is used.

5.3.2.1 Supersonic Case

The supersonic case is simple in the sense that the four homogeneous boundary conditions are imposed on the outflow boundary (table 7).

Table 7: Adjoint conditions and compatibility relations at the supersonic outlet

Characteristics entering the domain	4
Characteristics leaving the domain	0
Imposed adjoint conditions	$\varphi_i _{s_o} = 0$ (5.16)
Numerical conditions/Compatibility relations	-

The adjoint variables at the ghost cells are simply:

$$\varphi_{i,ghost}^{n+1} = \varphi_{i,ghost}^n = 0 \quad (5.17)$$

5.3.2.2 Subsonic Case

Three boundary conditions are imposed on the outflow boundary. They are given by equations (4.69), when solving the term (IIIb). To complete the set of properties at the ghost cells one can use the third compatibility relation of the characteristic adjoint equations. These equations are rewritten in table 8.

To solve the set of equations presented one can differentiate the imposed adjoint conditions with respect to time:

Table 8: Adjoint conditions and compatibility relations at the subsonic outlet

Characteristics entering the domain	3
Characteristics leaving the domain	1
Imposed adjoint conditions	$\begin{aligned}\varphi_1 &= C_1 \varphi_4 \\ \varphi_2 &= C_2 \varphi_4 \\ \varphi_3 &= C_3 \varphi_4\end{aligned}$
Numerical conditions/Compatibility relations	$K_{31}^t \frac{\partial \varphi_1}{\partial t} + K_{32}^t \frac{\partial \varphi_2}{\partial t} + K_{33}^t \frac{\partial \varphi_3}{\partial t} + K_{34}^t \frac{\partial \varphi_4}{\partial t} = R_3$

$$\begin{cases} \frac{\partial \varphi_1}{\partial t^*} - \frac{\partial C_1}{\partial t^*} \varphi_4 - C_1 \frac{\partial \varphi_4}{\partial t^*} = 0 \\ \frac{\partial \varphi_2}{\partial t^*} - \frac{\partial C_2}{\partial t^*} \varphi_4 - C_2 \frac{\partial \varphi_4}{\partial t^*} = 0 \\ \frac{\partial \varphi_3}{\partial t^*} - \frac{\partial C_3}{\partial t^*} \varphi_4 - C_3 \frac{\partial \varphi_4}{\partial t^*} = 0 \\ \left(\sum_{\beta=1}^3 K_{3\beta}^{t^*} C_\beta + K_{34}^{t^*} \right) \frac{\partial \varphi_4}{\partial t^*} = R_3 \end{cases} \quad (5.18)$$

As one is interesting in the transient, terms $\frac{\partial C_i}{\partial t^*}$ must be accounted for. The simplest way to compute them is by an approximation by finite differences, thus recovering the expression that is used for the subsonic inlet:

$$\frac{\partial C_i}{\partial t^*} \approx \frac{C_i(t^* + \Delta t^*) - C_i(t^* - \Delta t^*)}{2\Delta t^*} \quad (5.19)$$

And the system in $\frac{\partial \varphi_i}{\partial t^*}$ becomes:

$$\begin{cases} \frac{\partial \varphi_1}{\partial t^*} - C_1 \frac{\partial \varphi_4}{\partial t^*} = \left[\frac{C_1(t^* + \Delta t^*) - C_1(t^* - \Delta t^*)}{2\Delta t^*} \right] \varphi_4(t^*) \\ \frac{\partial \varphi_2}{\partial t^*} - C_2 \frac{\partial \varphi_4}{\partial t^*} = \left[\frac{C_2(t^* + \Delta t^*) - C_2(t^* - \Delta t^*)}{2\Delta t^*} \right] \varphi_4(t^*) \\ \frac{\partial \varphi_3}{\partial t^*} - C_3 \frac{\partial \varphi_4}{\partial t^*} = \left[\frac{C_3(t^* + \Delta t^*) - C_3(t^* - \Delta t^*)}{2\Delta t^*} \right] \varphi_4(t^*) \\ \left(\sum_{\beta=1}^3 K_{3\beta}^{t^*} C_\beta + K_{34}^{t^*} \right) \frac{\partial \varphi_4}{\partial t^*} = R_3 \end{cases} \quad (5.20)$$

On solving the set, the ghost cells adjoint variables are:

$$\varphi_{i,ghost}^{n+1} = \varphi_{i,ghost}^n + \frac{\partial \varphi_i}{\partial t^*} \Delta t \quad (5.21)$$

5.3.3 Solid Wall

The condition at the solid wall comes from equation (4.78). Since the property at a cell's edge is defined by the mean of the values at the adjacent elements, the discretized form of (4.78) is given by equation (5.22).

$$k_x \frac{\varphi_2^+ + \varphi_2^-}{2} + k_y \frac{\varphi_3^+ + \varphi_3^-}{2} = \frac{\partial \mathcal{F}}{\partial p} \sqrt{g_{11}} \quad (5.22)$$

Where the superscript $-$ refers to the ghost cells and the superscript $+$ refers to the cells at the interior domain.

From (5.22) it is noticed that a combination of φ_2^- and φ_3^- satisfying the equality is not unique. Therefore, the scheme used in the present work is the one presented by Reuther (1996) [3]:

$$\begin{cases} \varphi_1^- = \varphi_1^+ \\ \varphi_2^- = \varphi_2^+ + \frac{2k_x}{k_x^2 + k_y^2} \left(\frac{\partial \mathcal{F}}{\partial p} \sqrt{g_{11}} - k_x \varphi_2^+ - k_y \varphi_3^+ \right) \\ \varphi_3^- = \varphi_3^+ + \frac{2k_y}{k_x^2 + k_y^2} \left(\frac{\partial \mathcal{F}}{\partial p} \sqrt{g_{11}} - k_x \varphi_2^+ - k_y \varphi_3^+ \right) \\ \varphi_4^- = \varphi_4^+ \end{cases} \quad (5.23)$$

6 NUMERICAL RESULTS

Some examples of application cases are studied in this section. The objective is to conceptually validate the development of the continuous adjoint method to compute non-geometric sensitivities in unsteady flows, as proposed in this work. The simulations were made using the code originally developed by Hayashi (2006 [35] and 2016 [33]) to solve the Euler's Equations by means of the finite volume method. The code was modified in order to extend its applications to unsteady flows, with time-dependant boundary conditions and allowing time integration of the gradients calculated by the adjoint method.

The results obtained by the adjoint method are confronted with the ones obtained by finite differences. The reference state that was used to scale and nondimensionalize the flow variables is presented on table 9 (Hayashi, 2006) [35].

Table 9: Reference conditions for air

Reference conditions for air			
Parameter	Symbol	Value	Unit
Specific Mass	ρ_{ref}	1.486	$\frac{P}{m^3}$
Reference Velocity	v_{ref}	320.44	$\frac{m}{s}$
Reference Temperatures	T_{ref}	357.77	K
Ratio of specific heats	γ	1.4	-
Gas Constant	R	287	$\frac{J}{kg \cdot K}$

6.1 Internal Flow: Divergent Nozzle

One of the simplest cases is the divergent nozzle, therefore it is taken to be an important primary example to the present studies. The mesh and the initial boundary conditions are similar to the ones in Hayashi (2016) [33], since that case has already been fully validated for the steady flow solution.

The geometry of the nozzle is given by $y = 0.3x^2 + 0.3$, with $0 \leq x \leq 1$ and symmetry line at $y = 0$. The mesh has 9002 triangular elements and it is presented in figure 3.

Figure 3: Divergent nozzle mesh

The chosen measure of merit is the lateral force at the interior surface of the nozzle integrated over time, given by:

$$L = \frac{1}{T} \int_{t_o}^{t_f} \int_{b_w} (-pn_y \cos \theta + pn_x \sin \theta) dS dt \quad (6.1)$$

The nozzle is symmetric in relation to the plane $y = 0$. The force is computed only on the upper half of the nozzle.

The boundary conditions at permeable boundaries can vary with time. For the two first cases studied, the static pressure (for supersonic flows) and the total pressure (for subsonic flows) at the inlet are the varying properties. They are written in function of time as:

$$\begin{aligned} p_{inlet} &= p_{initial} + A \cdot p_{initial} \sin \omega t \quad (\text{supersonic case}) \\ p_{o,inlet} &= p_{o,initial} + B \cdot p_{o,initial} \sin \omega t \quad (\text{subsonic case}) \end{aligned} \quad (6.2)$$

In these cases $p_{inlet} = p[a_k = (p_{initial}, \omega, A)]$ (analogously for $p_{o,inlet}$), meaning that one can consider ω as a control parameter. Hence, the aim of the simulation is to compute $\frac{\partial I}{\partial a_k} = \frac{\partial L}{\partial \omega}$. Notice that if the inlet pressure were considered constant, one would go back to the case of Hayashi (2016) [33]. Although some of the chosen functions in this work are sinusoidal, it is evident that the method can be applied to other types of functions.

6.1.1 Supersonic Case

To compute the adjoint solution, one needs the time history of the physical solution. It is important to notice that the flow initial condition has to be physically possible. Thus, before the unsteady flow simulation, a steady-state solution is computed. The supersonic case requires that all the inflow conditions be imposed, while the outflow ones are free. The inlet conditions for the steady-state simulation are on table 10 and are the same as in the work of Hayashi (2016) [33].

Table 10: Inlet initial conditions for supersonic flow

Inlet Conditions	
Mach	2.0
Pressure	108987.7728 Pa
Temperature	255.556 K
Inlet Angle	0.0

The steady-state solution for the supersonic case is shown at figure 4. It is clear that the results are consistent with the ones obtained from Hayashi (2016) [33]. Evidently, the alterations made in the original code should not alter the simulations for the steady-state case. To ensure the results, the residues were computed and presented in table 11 to show the convergence of the steady solution.

Table 11: Residues for steady subsonic flow

Residues	
Mass	6.348691e-13
Momentum-x	1.567957e-12
Momentum-y	5.791677e-13
Energy	4.103139e-12

Once the steady-state for the given boundary conditions is obtained, it is possible to simulate the unsteady flow starting from the steady-state as initial condition. The inlet conditions remain the same with the exception of the static pressure, which is given by equation (6.2) and presented in the figure 5.

(a) Supersonic divergent nozzle initial condition: Mach

(b) Supersonic divergent nozzle initial condition: Pressure

(c) Supersonic divergent nozzle initial condition: Temperature

Figure 4: Supersonic divergent nozzle: steady-state initial condition

Figure 5: Inlet static pressure for different frequencies

Figure 6 shows the solution for the Mach number and pressure at specific time steps; the inflow pressure has the non-dimensional frequency $\omega = 15$. The non-dimensional period of simulation is $T \approx 0.53$ and each time step corresponds to $\Delta t \approx 0.001054$. As the inlet pressure changes in a sinusoidal fashion, it is possible to notice oscillating regions in the domain.

With the physical solution obtained, the adjoint equations are solved. It is emphasized that the initial condition is given by the homogeneous one, as described in the previous sections. Also, the time marching is reverse in relation to the physical one. The physical properties used to compute the adjoint solution at time t^* are taken from the physical solution at the corresponding time $t = T - t^*$. Figure 7 shows the adjoint state vector components Ψ_1 and Ψ_3 .

(a) Mach at $t \approx 0.052$ (b) Pressure at $t \approx 0.052$ (c) Mach at $t \approx 0.21$ (d) Pressure at $t \approx 0.21$ (e) Mach at $t \approx 0.37$ (f) Pressure at $t \approx 0.37$ Figure 6: Supersonic divergent nozzle: unsteady solution for frequency $\omega = 15$

Figure 7: Supersonic divergent nozzle: unsteady adjoint solution for $\omega = 15$ (obs: with time step referring to t^*)

Finally, once the physical and adjoint solutions are obtained, one can compute the derivative of the lateral force with respect to the control parameter. In this case, the inlet pressure is considered to be controlled by the oscillation frequency ω . The result is shown in figure 8. The sensitivity is computed by both the adjoint method and the finite differences.

Figure 8: Sensitivity of I with respect to the oscillation frequency ω of the inlet pressure (supersonic case) and $A = 0.15$

The figure shows agreement between the two methods (adjoint method and finite difference) and coherence of the values. The relative error computed based on the values from the FD method are between 2% and 4% with exception of the last point ($\omega = 15$). For this point, the adjoint method and the finite difference presented values close to zero ($O(10^{-6})$) as compared to the other points ($O(10^{-3})$), which incurred larger errors. It is possible that the sensitivity of the function of merit at that point be sufficiently small so the accuracy of the approximated numerical solution or the integration of the gradient over the time are not good enough to compute the value precisely.

6.1.2 Subsonic Case

Three physical conditions at the inlet and one at the outlet are required for the subsonic case. The initial condition at t_0 is given by the steady-state flow with the boundary conditions given by tables 12 and 13 (Hayashi, 2016) [33]. The period of simulation is $T \approx 0.4$ and each time step corresponds to $\Delta t \approx 0.000795$.

Table 12: Inlet initial conditions for subsonic flow

Inlet Conditions (non-dimension)	
Total Pressure	1.01
Total Temperature	0.75
Inlet Angle	0.0

Table 13: Outlet initial condition for subsonic flow

Outlet Conditions (non-dimension)	
Pressure	0.95

The steady flow solution for the Mach number, temperature and pressure are given in figure 9. Again, they are compatible with Hayashi (2016) [33] and the convergence of the solution is validated by table 14.

Table 14: Residues for steady subsonic flow

Residues	
Mass	4.458080e-13
Momentum-x	2.595671e-13
Momentum-y	3.222665e-13
Energy	9.963829e-13

Starting from the steady solution, the stagnation pressure at the inlet starts to change in time according to equation (6.2). The unsteady solution with oscillating boundary condition exhibits the behaviour illustrated in figure 10. In the subsonic case, the stagnation pressure is controlled but not the static pressure. The stagnation temperature and the inlet angle are kept constant, as well as the static pressure at the outlet.

(a) Subsonic divergent nozzle initial condition: Mach

(b) Subsonic divergent nozzle initial condition: Pressure

(c) Subsonic divergent nozzle initial condition: Temperature

Figure 9: Subsonic divergent nozzle: steady-state initial condition

(a) Mach at $t \approx 0.039$ (b) Pressure at $t \approx 0.039$ (c) Mach at $t \approx 0.16$ (d) Pressure at $t \approx 0.16$ (e) Mach at $t \approx 0.28$ (f) Pressure at $t \approx 0.28$ Figure 10: Subsonic divergent nozzle: unsteady solution for $\omega = 15$

The physical solution stored at each time step is used to compute the adjoint solution. The components Ψ_1 and Ψ_3 are illustrated in figure 11 at different time frames. The images corresponds to the reverse time t^* . Again, the initial adjoint condition is given by a null homogeneous field.

Figure 11: Subsonic divergent nozzle: unsteady adjoint solution for $\omega = 15$

The sensitivity of the lateral force on the interior surface of the nozzle with respect to the oscillation ω of the stagnation pressure at the inlet is given by figure 12. The values obtained by finite differences are also presented for comparison.

Figure 12: Sensitivity of I with respect to the oscillation frequency ω of the inlet total pressure (subsonic case) and $A = 0.15$

The points obtained from the two methods are coherent. The relative error was between 1% and 6% for many of the points. The point with the largest relative error was the last one ($\omega = 20$). It presented approximately 8% of error.

The subsonic case required the implementation of more complicated boundary conditions than those that are imposed on supersonic flows, as discussed previously. The statement is applied to both the physical and adjoint problems. However, the results of the adjoint method are in agreement with the finite difference.

6.2 Internal Flow: Convergent-Divergent Nozzle

A second geometry for an internal flow is studied in this section. In order to deepen the study of the proposed approach, a convergent-divergent nozzle (Laval nozzle) is simulated. Both the inlet and outlet are subsonic, however the flow reaches a supersonic regime at the throat and a normal shock is formed at the divergent section of the nozzle. Different cases are tested according to the type of boundary which is controlled (inlet or outlet). The stagnation pressure at the inlet and the static pressure at the outlet vary as equations (6.3). The measure of merit is still given by equation (6.1) and the mesh designed has approximately 20.000 triangular elements as figure 13 shows.

$$\begin{aligned} p_{o,inlet} &= p_{o,initial} + A \cdot t \quad (\text{case 1: inlet control}) \\ p_{outlet} &= p_{initial} + A \cdot t \quad (\text{case 2: outlet control}) \end{aligned} \tag{6.3}$$

Figure 13: Convergent-divergent nozzle mesh

The steady-state solution is computed with the boundary conditions in tables 15 and 16. As the inlet and outlet are subsonic, the required physical conditions to be imposed are: stagnation pressure, stagnation temperature, inlet angle at the inlet and static pressure at the outlet.

Table 15: Inlet initial conditions for the convergent-divergent nozzle

Inlet Conditions (non-dimension)	
Total Pressure	1.166
Total Temperature	0.75
Inlet Angle	0.0

Table 16: Outlet initial condition for the convergent-divergent nozzle

Outlet Conditions (non-dimension)	
Pressure	0.85

The converged solution of the steady state simulation is used as initial condition for the time-dependent problem. The residues are presented in table 17.

Table 17: Residues for steady subsonic flow: convergent-divergent nozzle

Residues	
Mass	5.513988e-13
Momentum-x	2.245459e-13
Momentum-y	1.313840e-13
Energy	9.785654e-13

Figure 14a shows the steady solution. The normal shock at the divergent section, where the Mach number abruptly decays from 1.5 to 0.7, and the non-dimensional pressure increases from 0.32 to 0.8 as expected.

The solution is set as initial condition to the unsteady simulation. From the instant t_0 the stagnation pressure starts to linearly increase. The simulation period is $T \approx 8$ (non-dimensional) and the time step is $\Delta t \approx 0.008$. Figure 14 shows the pressure distribution at the initial condition $t = 0$, $t \approx 4$ and $t \approx 8$ for $A \approx 0.03$. One can notice the increasing pressure at the nozzle. Figures 15 and 16 show the adjoint solution for Ψ_1 and Ψ_3 at the reverse time frames $t^* = T - t \approx 4$ and $t^* \approx 8$. The derivative $\frac{\partial I}{\partial \omega}$ is computed with both the physical and adjoint solutions.

(a) Pressure at $t = 0$ (initial condition) (b) Pressure at $t \approx 4$ (c) Pressure at $t \approx 8$

Figure 14: Convergent-divergent nozzle: unsteady solution for increasing stagnation pressure at the inlet

(a) Ψ_1 at $t^* \approx 4$ (b) Ψ_1 at $t^* \approx 8$ Figure 15: Convergent-divergent nozzle: adjoint solution Ψ_1

(a) Ψ_3 at $t^* \approx 4$ (b) Ψ_3 at $t^* \approx 8$ Figure 16: Convergent-divergent nozzle: adjoint solution Ψ_3

The derivative of the lateral force integrated in time with respect to the rate with which the inlet stagnation pressure increases is presented in Figure 17. The results obtained from the adjoint method and the finite differences are compared.

Figure 17: Sensitivity of I with respect to the rate A of the inlet stagnation pressure (subsonic case)

The results show little variation of the sensitivity $\partial I / \partial A$ with the change of the control parameter A . The values obtained from the different methods have relative errors between 1% and 3%. The presence of the shock wave inside the domain does not change the mathematical formulation proposed, however the accuracy of the numerical solution may have a great impact on the results due to the substantial gradients suffered by the flow. Besides, the location of the discontinuity and the size of the mesh elements can also have a major effect. Yet, the agreement of the values in this case are expressive.

The second case concerns the study of the adjoint method to compute sensitivities at the outlet. There is only one physical boundary condition required at the subsonic outlet, which is the static pressure for the present simulation. The static pressure varies linearly with time. Figure 18 presents the compared values of $\partial I / \partial A$.

Figure 18: Sensitivity of I with respect to the rate A of the outlet static pressure (subsonic case)

The time of simulation was $T \approx 4$. Similarly to the controlled inlet case, the values of $\partial I / \partial A$ have little change with respect to A . The relative error between the adjoint method and finite differences was approximately 4.5%. The results are in agreement with the expected from the finite differences method. Some remarks are made: although the coherent results, the relative error compared to the inlet test case are greater; the facts that the information of change in pressure at the outlet propagates against the flow velocity and the proximity of the shock wave from the outlet seem to cause disturbances in the flow with higher spatial gradients than the inlet case; the information can not propagates besides the shock wave as the Mach number in the section before the shock is greater than 1.

One final case is simulated for a time $T \approx 4$. As made for the divergent nozzle, the inlet stagnation pressure is assumed to be controlled and its described value is given by equation (6.4).

$$p_{o,inlet} = p_{o,initial} + A \cdot p_{o,initial} \sin \omega t \quad (6.4)$$

In order to illustrate this case, Figure 19 shows the stagnation pressure for $\omega = 5$ at times $t = 0$ and $t \approx 4$.

(a) Stagnation pressure at $t = 0$

(b) Stagnation pressure at $t \approx 4$

Figure 19: Stagnation pressure for $\omega = 5$

As the flow is modelled by the Euler's equations in this work, there is no physical viscosity (although there is a numerical dissipation). At $t = 0$, the stagnation pressure, which is directly associated to the entropy level, is constant and homogeneous until the shock wave, decaying abruptly as expected. The stagnation pressure starts to oscillate causing the waves presented in Figure 19.

The values of the sensitivity $\partial I / \partial \omega$ are plotted in Figure 20.

Figure 20: Sensitivity of I with respect to the oscillation frequency ω of the inlet stagnation pressure (subsonic case) and $A = 0.02$

The sensitivity computed by the adjoint method is in agreement with the finite differences. Although still simple, the proposed case presents a more complex variation at the boundary than the precedent cases. Therefore, it is expected that the solution be more complex as well. The relative error remained approximately at 4%. However, the points obtained for the frequency $\omega = 2.5$ and $\omega = 4$ were in less agreement between the methods, with relative error of 19% and 45%. These points have small values compared to the others obtained (in particular, the point for $\omega = 4$ has magnitude of order $O(10^{-4})$).

It should be remarked from the cases exposed that the mesh used is still coarse but, unfortunately, there is a substantial computational cost to save the solution at each time step. Besides, the code used is relatively simple and not optimized. Therefore, it was tried to achieve balance between the number of elements, time steps and accuracy of the numerical solution, in order to have enough resolution to validate the method proposed. The goal of this work is not to pursue best accuracy but rather study the validation of the mathematical development.

6.3 External Flow: RAE 2822

The approach developed in this work to compute adjoint based sensitivities with respect to non-geometric parameters holds for both internal and external aerodynamics. Its flexibility is tested in this section for external flows over an airfoil with profile RAE 2822. The flow regime considered is supersonic. The mesh used is presented in figures 21 and 22. Figure 21 shows the entire domain, while figure 22 zooms the mesh over the airfoil.

All the characteristics travel from the inlet to the outlet in the supersonic case, consequently, no information propagates backwards. It can be used as an advantage to restrict the distance between the airfoil and the inlet.

Figure 21: RAE 2822 mesh

Figure 22: RAE 2822 mesh at the airfoil

The measure of merit is similar to the ones previously used, however it represents the non-dimensional lift:

$$L = \frac{1}{T} \int_{t_o}^{t_f} \int_{b_w} (-pn_y \cos \theta + pn_x \sin \theta) dS dt \quad (6.5)$$

The x-component of the velocity at the inlet varies linearly with the time:

$$u = u_{initial} + a \cdot t \quad (6.6)$$

Naturally, the control parameters are $a_k = (u_{initial}, a)$.

Boundary conditions for the steady state solution are described in table 18. Again, as the flow is supersonic, all characteristics at the inlet travel from the outside to the inside of the domain, therefore, four properties must be selected as boundary conditions. At the outlet all the characteristic are leaving the domain, in other words, the properties at the outlet are totally determined from the solution. Notice that it is totally equal to the internal flow.

Table 18: Inlet initial conditions for supersonic flow over a RAE 2822 profile

Inlet Conditions	
Mach	1.4
Pressure	108987.7728 Pa
Temperature	255.556 K
Inlet Angle	3°

One can notice that the four properties chosen in the mathematical development were ρ , u , v and p . With the exception of the pressure, the other properties are not listed in table 18. The explanation is that, from the initial properties in the table, the other ones are computed and, then, set as the imposed ones.

The converged solution set as initial condition has the residues indicated below:

Table 19: Residues for steady supersonic flow over a NACA 0012 profile

Residues	
Mass	5.203111e-12
Momentum-x	9.806107e-12
Momentum-y	3.657102e-12
Energy	1.440320e-11

The Mach number and pressure distribution of the solution are presented in figures 23 and 24. As expected, there is a detached shock wave near the leading edge. The time-dependent simulation starts from the steady-state solution and the x-component of the velocity at the inlet increases linearly.

(a) Supersonic RAE 2822 initial condition: Mach

(b) Supersonic RAE 2822 at $t \approx 1.45$: Mach

Figure 23: Supersonic RAE 2822 - Mach

(a) Supersonic RAE 2822 initial condition: Pressure

(b) Supersonic RAE 2822 at $t \approx 1.45$: Pressure

Figure 24: Supersonic RAE 2822 - Pressure

The non-dimensional simulation period was $T \approx 1.45$ with the time step $\Delta t \approx 1.6 \cdot 10^{-4}$. The information travels at a limited speed through the domain, consequently, it takes some time until the change of pressure at the farfield reaches the airfoil. Due to the great distance the information has to travel, the time simulated is also increased.

The adjoint solution Ψ_1 is presented in figure 25 at two different time frames for the control parameter $a = 0.12$. Figure 26 shows the same for Ψ_3 . It is interesting to observe how the adjoint solution does travel in the opposite direction to the flow solution.

(a) Supersonic RAE 2822: Ψ_1 at $t^* \approx 0.72$ (b) Supersonic RAE 2822: Ψ_1 at $t^* \approx 1.45$ Figure 25: Supersonic RAE 2822 - adjoint solution Ψ_1

(a) Supersonic RAE 2822: Ψ_3 at $t^* \approx 0.72$ (b) Supersonic RAE 2822: Ψ_3 at $t^* \approx 1.45$ Figure 26: Supersonic RAE 2822 - adjoint solution Ψ_3

The derivative of the measure of merit with respect to the rate of decrease in pressure is computed using the adjoint method and the finite difference approach. The results are in figure 27.

Figure 27: Sensitivity of I with respect to the slope a of the inlet pressure (supersonic case)

The results have an average relative error around 5%. Although the values obtained from the adjoint method are smaller than the ones obtained from the finite difference, the comparison between them shows reasonable agreement.

7 CONCLUSION

The continuous adjoint method that is usually applied to compute geometric derivatives in aerodynamics was extended to provide an alternative tool to compute non-geometric derivatives in time-dependent flows. The adjoint boundary conditions were derived to guarantee that the adjoint problem is as well-posed as the physical problem.

The test cases simulated in this work show the agreement between the sensitivity gradients computed with the proposed method and the finite differences approach. In particular, some of the results obtained with the subsonic divergent nozzle and convergent-divergent nozzle with controlled inlet presented less than 3% of error. Evidently, the meshes used can be refined and the precision and accuracy of the numerical methods can be improved, however, the present work has the sole purpose of deriving and validating the proposed approach.

Although the simulations were rather simple, they can represent some interesting problems. For instance, a convergent-divergent nozzle can represent the nozzle of a rocket ascending the atmosphere. The outlet pressure decreases when the altitude increases and a study of the sensitivity gradients can be computed with respect to the speed with which the rocket travels. The Laval nozzle can also represent a wind tunnel, if the nozzle is connected to a reservoir with variable pressure or temperature, one can analyze the behaviour of the flow according to the variation of the properties at the reservoir. For external flows, two potential applications are flight dynamics and aeroelasticity, since the method can be used to compute stability derivatives.

From the theoretical point of view, the appropriate study of the boundary conditions of the adjoint problem is less explored in the literature. The present work tries to explore this subject in order to establish a coherent method. Again, some important facts are worth mentioning: the proposed method can be equally applied to internal and external flows; the initial condition set for the time-dependent simulation is computed as the solution of a steady-state flow, this guarantees that the initial condition belongs to the space of realizable flows; starting from this condition, the gradient of the time-averaged

functional can be computed for an arbitrary time (as long as the solution is time accurate); the adjoint solution depends on the physical solution at each corresponding time step, therefore, the latter one needs to be saved entirely (or it must contain enough information for its reconstruction). In that regard, it should be noted that the computational cost the method incurs can be very significant. However, it is important to add that it makes use of the very same adjoint continuous formulation that is applied to geometric sensitivities. Therefore, it does not imply any rise in computational costs over the latter, when both kinds of sensitivities, geometric and otherwise are computed for the same class of flows.

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APPENDIX A – COEFFICIENTS OF THE CHARACTERISTIC ADJOINT EQUATION

$$K^{t*} = \begin{bmatrix} 1 & u & v & \frac{u^2+v^2}{2} \\ 0 & \rho k_y & -\rho k_x & \rho(k_y u - k_x v) \\ \rho & \rho(u + k_x c) & \rho(v + k_y c) & \frac{\rho c^2}{\gamma-1} + \rho c(k_x u + k_y v) + \frac{\rho}{2}(u^2 + v^2) \\ \rho & \rho(u - k_x c) & \rho(v - k_y c) & \frac{\rho c^2}{\gamma-1} - \rho c(k_x u + k_y v) + \frac{\rho}{2}(u^2 + v^2) \end{bmatrix} \quad (\text{A.1})$$

$$K^x = \begin{bmatrix} u & u^2 & uv \\ \rho k_y & 2\rho k_y u & -\rho(k_x u - k_y v) \\ \rho(u + k_x c) & \rho c^2 k_y^2 + \rho(u + k_x c)^2 & -[\rho c^2 k_x k_y - \rho(u + k_x c)(v + k_y c)] \\ \rho(u - k_x c) & \rho c^2 k_y^2 + \rho(u - k_x c)^2 & -[\rho c^2 k_x k_y - \rho(u - k_x c)(v - k_y c)] \\ \frac{u(u^2+v^2)}{2} & & \\ -\left[\rho k_x uv - \frac{\rho k_y(3u^2+v^2)}{2} - \frac{\rho c^2 k_y}{\gamma-1}\right] & & \\ -\left[\rho c^2 k_y(k_x v - k_y u) - \frac{\rho}{2}(u + k_x c)(u^2 + v^2) - \rho c(u + k_x c)(k_x u + k_y v) - \frac{\rho c^2(u+k_x c)}{\gamma-1}\right] & & \\ \left[\rho c^2 k_y(k_x v - k_y u) + \frac{\rho}{2}(u - k_x c)(u^2 + v^2) - \rho c(u + k_x c)(k_x u + k_y v) + \frac{\rho c^2(u-k_x c)}{\gamma-1}\right] & & \end{bmatrix} \quad (\text{A.2})$$

$$K^y = \begin{bmatrix} v & uv & v^2 \\ -\rho k_x & -\rho(k_x u - k_y v) & -2\rho k_x v \\ \rho(v + k_y c) & -[\rho c^2 k_x k_y - \rho(u + k_x c)(v + k_y c)] & \rho c^2 k_x^2 + \rho(v + k_y c)^2 \\ \rho(v - k_y c) & -[\rho c^2 k_x k_y + \rho(u - k_x c)(v - k_y c)] & \rho c^2 k_x^2 - \rho(v - k_y c)^2 \\ \frac{v(u^2 + v^2)}{2} & \left[\rho k_y uv - \frac{\rho k_x(u^2 + 3v^2)}{2} - \frac{\rho c^2 k_x}{\gamma - 1} \right] & \\ -\left[\rho c^2 k_x(k_y u - k_x v) - \frac{\rho}{2}(v + k_y c)(u^2 + v^2) - \rho c(v + k_y c)(k_x u + k_y v) - \frac{\rho c^2(v + k_y c)}{\gamma - 1} \right] & & \\ -\left[\rho c^2 k_x(k_y u - k_x v) - \frac{\rho}{2}(v - k_y c)(u^2 + v^2) + \rho c(v - k_y c)(k_x u + k_y v) - \frac{\rho c^2(v - k_y c)}{\gamma - 1} \right] & & \end{bmatrix} \quad (\text{A.3})$$