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Analysis of finite-volume discrete adjoint fields for two-dimensional compressible Euler flows

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Abstract

This work deals with a number of questions related to the discrete and continuous adjoint fields associated with the compressible Euler equations and classical aerodynamic functions. The consistency of the discrete adjoint equations with the corresponding continuous adjoint partial differential equations is one of them. It is has been established or at least discussed only for some numerical schemes and a contribution of this article is to give the adjoint consistency conditions for the 2-D Jameson-Schmidt-Turkel scheme in cell-centred finite-volume formulation. The consistency issue is also studied here from a new heuristic point of view by discretizing the continuous adjoint equation for the discrete flow and adjoint fields. Both points of view prove to provide useful information. Besides, it has been often noted that discrete or continuous inviscid lift and drag adjoint exhibit numerical divergence close to the wall and stagnation streamline for a wide range of subsonic and transonic flow conditions. This is analyzed here using the physical source term perturbation method introduced in reference [1]. With this point of view, the fourth physical source term of [1] appears to be the only one responsible for this behavior. It is also demonstrated that the numerical divergence of the adjoint variables corresponds to the response of the flow to the convected increment of stagnation pressure and diminution of entropy created at the source and the resulting change in lift and drag.

Keywords: discrete adjoint method, continuous adjoint method, dual consistency, compressible Euler equations, adjoint Rankine-Hugoniot relation

1. Introduction

Discrete and continuous adjoint methods are well established methods to efficiently calculate derivatives of aerodynamic functions with respect to numerous design parameters. Adjoint-based derivatives and adjoint-fields are commonly used for local shape optimization [2, 3, 4, 5, 6], goal-oriented mesh adaptation [7, 8, 9, 10, 11, 12, 13, 14], flow control [15, 16], meta-modelling [17], receptivity-sensitivity-stability analyses [18], and data assimilation [19]. These methods are often used for the linear analysis of non-linear conservation laws where the adjoint is defined as the dual to the linearized equations around a given solution to the direct non-linear problem. The continuous adjoint method refers to the discretization of the adjoint equations associated with the formal direct problem, while the discrete adjoint method refers to the adjoint equations to the discrete direct problem. The advantages and disavantages of the two approaches have been listed in several articles [20, 21].

Concerning the discrete adjoint method, strong efforts have been devoted to implement (either by hand or using automatic differentiation) the exact linearization of intricate schemes for intricate models [22, 23] and to enhance the robustness of the linear solver [24, 25]. However fundamental questions related to the discrete adjoint fields are still open even for two-dimensional (2-D) compressible Euler flows. Although numerical simulations including viscous laminar and turbulent effects are currently common practices in CFD, it is desirable to gain a further understanding in the discrete adjoint method addressing unresolved questions in the framework of 2-D Euler equations.

First, are the discrete adjoint fields consistent with the continuous equation at the limit of fine meshes? This subject goes back to a discussion by Giles et al. in [26] where the authors discussed the discrete adjoint counterpart of a strong

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boundary condition at a wall and derived a normal projection of the momentum adjoint variable that did not correspond to the normal momentum component of the continuous adjoint solution at the boundary. Although, of course, the exact discrete adjoint provides the exact output functional gradient for a fixed mesh and scheme, this oddness raised a series of questions: which schemes are adjoint-consistent? What are the consequences of the lack of dual consistency? How close are continuous adjoints and possibly inconsistent discrete adjoints? These points have been addressed using numerical comparisons by Nadarajah and Jameson who also discussed the influence of the adjoint gradient accuracy on the final optimized shapes for airfoil design problems [27, 28]. Neither the discrepancy in the gradients, nor the difference in the final shapes they observed on intermediate and coarse meshes were very significant. Nevertheless it is sound to gain a more general understanding in this area. The adjoint consistency issue in CFD has also been studied theoretically in some articles where the authors have to first precisely describe the numerical method they consider, including the possibly specific discretization close to the boundary, and also the way the function of interest is discretized. Lu and Darmofal [29] considered a discontinuous Galerkin (DG) scheme and then demonstrated how to formulate the primal boundary condition and the output functional to obtain dual consistency. The difference between the consistent and non consistent formulations is noticed in both the appearance of spurious oscillations in the adjoint contours close to the function support and the convergence rate of the output of interest w.r.t. the characteristic mesh size. Hartmann [30] also discussed dual consistency for DG schemes, including interior penalty DG and also dealt with Navier-Stokes equations and test-cases. The adjoint consistency of a high-order correction procedure via reconstruction formulation for hyperbolic conservation laws was investigated in [31]. As concerning finite-differences and finite-volume (FV), the questions of adjoint consistency was discussed by Duivesteijn et al. and Lozano for quasi-one-dimensional Euler flows [32, 33] and also for an unsteady conservation law by Liu and Sandu [34]. In this later article, the authors considered first-order and second-order upwind schemes and derived the circumstances in which the discrete adjoint is punctually not consistent (change of convection direction, inadequate discretization of boundary condition in particular). Hicken and Zingg have demonstrated the influence of adjoint consistency for a class of summation-by-parts difference schemes, illustrating the benefit of consistency in terms of regularity of adjoint contours close to boundaries, functional grid-convergence, and dual-weighted corrected functional mesh convergence [35]. Recently, Stück carried out a corresponding effort for cell-vertex FV discretization (using median dual grids), deriving the condition on the output of interest and scheme residual for dual consistency [36, 37]. In this article, the conditions for dual consistency of the classical Jameson-Schmidt-Turkel (JST) scheme in 2-D cell-centered FV are derived. Besides, the dual consistency is also studied here from a heuristic point of view, discretizing the continuous adjoint equation for the discrete adjoint fields which adds valuable information to the theoretical study where the flow or the gradient of the adjoint is discontinuous and where numerical divergence of the adjoint is observed

In the case of hyperbolic equations, the validity of the adjoint linearization around discontinuities in the direct solution has to be carefully handled because it results in linear equations with discontinuous coefficients. The analysis must include the linearization of the jump relations at the discontinuity [38] which leads to a so-called interior boundary condition for the adjoint variables [39]. The adjoint relations to the Rankine-Hugoniot (RH) relations have been derived in [40] for the quasi-one-dimensional and in [41, 42] for the 2-D compressible Euler equations and proved continuity of the adjoint variables across the shock. In contrast, their derivatives may be discontinuous [40, 1, 41]. Lozano [42] also briefly discussed the consistency of the continuous adjoint fields but on rather coarse meshes. The conclusions of his work leave the question open whether these relations are actually satisfied at the limit of fine discrete adjoint fields.

Finally, it has been well-documented [1, 43, 42, 44] that, at certain flow conditions, the inviscid lift and drag adjoint fields may exhibit increasing values as the mesh is refined close to the stagnation streamline, the wall and, for (at least locally) supersonic flows, the Mach lines impacting a shock foot. In the case of the stagnation line, Giles and Pierce derived a $1/\sqrt{d}$ law for lift and drag adjoint [1] (d being the distance to the line), but they used the potential flow theory and this $1/\sqrt{d}$ behavior is not always well-observed for compressible flows [43, 42]. In an effort to analyze the zones of singular behavior, Todarello et al. [45] used the characterization of the discrete adjoint and looked how the flow is perturbed by a residual perturbation located in one of the these specific areas. This method is used again here but with perturbations of the residual corresponding to physical source terms [1] which allows fluid mechanics analysis. In this framework, it appears that the numerical divergence of the adjoint variables close to the stagnation streamline and the wall is due to the influence of the fourth of the source term proposed in [1], the corresponding convected increment of stagnation pressure and diminution of entropy (created at the location of the source) and the resulting change in lift and drag. Finally, some other aspects of 2-D inviscid lift and drag adjoint field are studied in

details. In particular, in the case of a supersonic flow with a detached shock wave, the mathematical expression of the adjoint field upwind the shock wave is derived.

The paper is organized as follows. Sections 2 and 3 are devoted to reminders about continuous and discrete adjoint solutions for compressible Euler flows. The adjoint consistency of the cell-centered JST scheme with structured 2-D meshes [46] is theoretically discussed in § 4. The theoretical results about adjoint consistency and adjoint-gradient discontinuity at shock waves are then assessed in § 5 using lift- and drag-adjoint fields for inviscid flows around the NACA0012 airfoil in supersonic (§ 5.2), transonic (§ 5.3) and subsonic (§ 5.4) regimes. The dual consistency property is then also practically discussed discretizing the continuous adjoint equation for fine grid discrete adjoint fields. This appears to highlight several zones of numerical divergence of the adjoint fields and this divergence is analysed in the vicinity of the wall and the stagnation streamline. Finally, concluding remarks about this work are given in § 6.

2. Continuous adjoint equations for 2-D Euler flows

2.1. Regions of smooth flow

The continuous adjoint equations for gas dynamics were first derived by Jameson [4] in the case of 2-D compressible Euler flows around a profile. He considered a body fitted structured grid that was mapped to a conformal rectangle and used the Euler equations in the resulting (ξ, η) -coordinates. A parametrization of the mapping then allowed to vary the airfoil shape in the physical space (without altering the domain of variation of the transformed coordinates) and to define a gradient calculation problem for functional outputs.

As, in this formulation, the system of transformed coordinates is attached to a structured mesh, the aforementioned equations could not be used for unstructured CFD for which a formulation in physical coordinates was necessary. The corresponding system of equations was first derived by Anderson and Venkatakrishnan in [47] and then by Hiernaux and Essers [48, 49]. Below we recall shortly the theory from [47].

The quantity of interest is assumed to be the projection of the force applied by the fluid onto the solid, projected in the direction $\overline{d} = (-\cos \alpha, \sin \alpha)^T$ for the lift, or $\overline{d} = (\sin \alpha, \cos \alpha)^T$ for drag with α the angle of attack:

$$J = \int_{\Gamma_w} p(\overline{n} \cdot \overline{d}) ds, \tag{1}$$

where Γ_w is the boundary of the solid body, $\overline{n} = (n_x, n_y)^T$ is the unit normal vector pointing outward, and p is the static pressure.

The 2-D steady compressible Euler equations in conservative form read

$$\frac{\partial F_x(W)}{\partial x} + \frac{\partial F_y(W)}{\partial y} = 0 \quad \text{in } \Omega,$$
(2)

W being the vector of conservative variables and F_x and F_y the physical fluxes:

$$W = \begin{pmatrix} \rho \\ \rho u_x \\ \rho u_y \\ \rho E \end{pmatrix}, \quad F_x(W) = \begin{pmatrix} \rho u_x \\ \rho u_x^2 + p \\ \rho u_x u_y \\ \rho u_x H \end{pmatrix}, \quad F_y(W) = \begin{pmatrix} \rho u_y \\ \rho u_y u_y \\ \rho u_y^2 + p \\ \rho u_y H \end{pmatrix},$$

with $H = E + p/\rho$ the total specific enthalpy and $\overline{U} = (u_x, u_y)^T$ the velocity vector. We assume an ideal gas law for the static pressure $p = (\gamma - 1)\rho e = (\gamma - 1)(\rho E - \frac{1}{2}\rho ||\overline{U}||^2)$ with γ the ratio of specific heats. Let δW by a perturbation in the steady state flow that is caused be an infinitesimal perturbation of the airfoil shape or flow conditions. As Wand $W + \delta W$ are solutions to the steady Euler equations for the initial and perturbed problems, we get by difference

$$\frac{\partial (A\delta W)}{\partial x} + \frac{\partial (B\delta W)}{\partial y} = 0 \quad \text{in } \Omega,$$

with A and B the Jacobians of the fluxes F_x and F_y , respectively. The perturbation in J can be augmented by the dot product of the above equation with an arbitrary co-state field ψ :

$$\delta J = \int_{\Gamma_w} \delta p(\overline{n} \cdot \overline{d}) ds + \int_{\Gamma_w} p(\delta(\overline{n}) \cdot \overline{d}) ds + \int_{\Gamma_w} p(\overline{n} \cdot \overline{d}) \delta(ds) + \int_{\Omega} \Psi^T \left(\frac{\partial (A \delta W)}{\partial x} + \frac{\partial (B \delta W)}{\partial y} \right) dv,$$
3

where at first order $\delta p = \nabla p \cdot \delta \mathbf{x} + \mathbf{p}'(\mathbf{W}) \cdot \delta \mathbf{W}$ represents pressure variations due to both geometry variations $\delta \mathbf{x} = (\delta x, \delta y)^T$ and solution variations $\delta \mathbf{W}$ due to this change in the geometry.

Assuming smooth direct and adjoint solutions, the last term can be transformed by integration by parts into

$$-\int_{\Omega}\left(\frac{\partial\psi^{T}}{\partial x}A+\frac{\partial\psi^{T}}{\partial y}B\right)\delta Wdv+\int_{\Gamma_{W}\cup\Gamma_{\infty}}\psi^{T}(n_{x}A+n_{y}B)\delta Wds$$

with Γ_{∞} the far field boundary, so we have

$$\delta J = \int_{\Gamma_w} \left(\delta p(\overline{n} \cdot \overline{d}) + \int_{\Gamma_w} p(\delta(\overline{n}) \cdot \overline{d}) \right) ds + p(\overline{n} \cdot \overline{d}) \delta(ds) - \int_{\Omega} \left(\frac{\partial \psi^T}{\partial x} A + \frac{\partial \psi^T}{\partial x} B \right) \delta W dv + \int_{\Gamma_w \cup \Gamma_\infty} \psi^T (n_x A + n_y B) \delta W ds$$
(3)

The adjoint method removes the dependency in the flow perturbation δW for the evaluation of the variation of J. This directly yields the adjoint equation in the fluid domain:

$$-A^{T}\frac{\partial\psi}{\partial x} - B^{T}\frac{\partial\psi}{\partial y} = 0, \quad \text{in } \Omega.$$
(4)

Note that manipulating (4) one may deduce

$$\overline{U} \cdot \nabla \psi_1 - H\overline{U} \cdot \nabla \psi_4 = 0. \tag{5}$$

Besides, using the variation of the boundary condition $\delta(\overline{U} \cdot \overline{n}) = 0$ and expanding $\psi^T(n_x A + n_y B)\delta W$ at the wall yields the wall boundary condition [47]

$$\bar{\imath} \cdot d + \psi_2 n_x + \psi_3 n_y = 0. \tag{6}$$

In the far field, no variation of the boundary needs to be considered. The Jacobian in direction \overline{n} can be rewritten by using a locally one-dimensional characteristic decomposition to yield

$$\int_{\Gamma_{\infty}} \Psi^T (n_x A + n_y B) \delta W ds = \int_{\Gamma_{\infty}} (\Psi^T P^{-1} D P \delta W) ds.$$
⁽⁷⁾

It is assumed that $P\delta W \simeq \delta(PW)$. The variation in these characteristic variables is zero for the components corresponding to negative eigenvalues of the Jacobian, $n_x A + n_y B$, in the classical 1D approximate linearization at the boundary (information coming from outside of the domain and fixed characteristic value). The far field adjoint BC simply imposes that the other components of $\psi^T P^{-1}$ are zero so that $\delta W^T (n_x A^T + n_y B^T) \psi$ vanishes for all δW .

2.2. Jump relations for the adjoint derivatives

We derive here some useful relations for the jump of the adjoint variables derivatives across the shock. As reported in the introduction, the derivation of the adjoint Rankine-Hugoniot relations for the quasi-one-dimensional [40] and 2-D [42, 41] compressible Euler equations show that the adjoint variables are continuous across the shock, while the adjoint derivatives in the direction normal to the shock may be discontinuous. These jump relations for the derivatives have been manipulated in [42] to provide information on the behavior of adjoint variables at shocks. We reproduce here this latter analysis but in a somewhat more general way and numerical experiments on very fine meshes in Figs. 7 and 12 will support our conclusions.

Let consider an isolated discontinuity Σ where the direct solution satisfies the RH jump relations

$$[[n_x F_x(W) + n_y F_y(W)]] = 0, (8)$$

where $[\![\cdot]\!]$ denotes the jump across Σ in the unit direction $\overline{n} = (n_x, n_y)^T$ normal to Σ . Introducing $\overline{t} = (-n_y, n_x)^T$, the adjoint equation (4) may be rewritten as

$$-A_n^T \frac{\partial \Psi}{\partial n} - A_t^T \frac{\partial \Psi}{\partial t} = 0 \quad \text{in } \Omega,$$
⁽⁹⁾

with

$$A_{n} = n_{x}A + n_{y}B = \begin{pmatrix} 0 & n_{x} & n_{y} & 0\\ (\gamma - 1)e_{c}n_{x} - uv_{n} & v_{n} - (\gamma - 2)un_{x} & un_{y} - (\gamma - 1)vn_{x} & (\gamma - 1)n_{x}\\ (\gamma - 1)e_{c}n_{y} - vv_{n} & vn_{x} - (\gamma - 1)un_{y} & v_{n} - (\gamma - 2)vn_{y} & (\gamma - 1)n_{y}\\ ((\gamma - 1)e_{c} - H)v_{n} & Hn_{x} - (\gamma - 1)uv_{n} & Hn_{y} - (\gamma - 1)vv_{n} & \gamma v_{n} \end{pmatrix},$$

$$A_{t} = -n_{y}A + n_{x}B = \begin{pmatrix} 0 & -n_{y} & n_{x} & 0\\ -(\gamma - 1)e_{c}n_{y} - uv_{t} & v_{t} + (\gamma - 2)un_{y} & un_{x} + (\gamma - 1)vn_{y} & -(\gamma - 1)n_{y}\\ (\gamma - 1)e_{c}n_{x} - vv_{t} & -vn_{y} - (\gamma - 1)un_{x} & v_{t} - (\gamma - 2)vn_{x} & (\gamma - 1)n_{x}\\ ((\gamma - 1)e_{c} - H)v_{t} & -Hn_{y} - (\gamma - 1)uv_{t} & Hn_{x} - (\gamma - 1)vv_{t} & \gamma v_{t} \end{pmatrix},$$

where $v_n = \overline{n} \cdot \overline{U}$, $v_t = \overline{t} \cdot \overline{U}$, $\partial_n \psi = n_x \partial_x \psi + n_y \partial_y \psi$, and $\partial_t \psi = -n_y \partial_x \psi + n_x \partial_y \psi$. Assuming that A_n is non-singular, the adjoint is continuous across Σ [40, 1, 42, 41]: $[\![\psi]\!] = 0$, so $[\![\partial_t \psi]\!] = 0$. Likewise we have $[\![\rho v_n]\!] = 0$, $[\![v_t]\!] = 0$, and $[\![H]\!] = 0$.

Let (9a-d) denote the four equations in (9). Then, the operation $(9a) + \frac{u_x}{2}(9b) + \frac{u_y}{2}(9c)$ gives

$$\frac{v_n}{2}(\partial_n\psi_1-H\partial_n\psi_4)+\frac{v_t}{2}(\partial_t\psi_1-H\partial_t\psi_4)=0,$$

and applying the jump operator we obtain

$$\llbracket v_n \partial_n \psi_1 \rrbracket - H \llbracket v_n \partial_n \psi_4 \rrbracket = 0. \tag{10}$$

Note that for functions of the static pressure and the geometry and uniform far field, one gets from (5) that $\nabla \psi_1 = H \nabla \psi_4$ which is actually observed later on in the numerical experiments with lift and drag adjoint (see also equation (18) below). Likewise, (9d) gives

$$(\gamma - 1) \llbracket n_x \partial_n \psi_2 + n_y \partial_n \psi_3 \rrbracket + \gamma \llbracket v_n \partial_n \psi_4 \rrbracket = 0, \tag{11}$$

and the operations $[[n_x(9c)-n_y(9b)]]$ and $[[n_x(9b)+n_y(9c)]]$ result in

$$[[v_n(-n_y\partial_n\psi_2+n_x\partial_n\psi_3+v_t\partial_n\psi_4)]]+[[v_n]](n_x\partial_t\psi_2+n_y\partial_t\psi_3)=0,$$
(12a)

$$[[\partial_n \psi_1]] + [[(u + v_n n_x)\partial_n \psi_2 + (v + v_n n_y)\partial_n \psi_3 + (H + v_n^2)\partial_n \psi_4]] + [[v_n]]v_t \partial_t \psi_4 = 0.$$
(12b)

Finally, the adjoint equation to the RH relations (8) reads $[[-n_y F_x(W) + n_x F_y(W)]] \cdot \partial_t \psi = 0$ [40, 42, 41] which may be simplified into

$$v_t[\![\rho]\!](\partial_t \psi_1 + H \partial_t \psi_4) + ([\![p]\!] + v_t^2[\![\rho]\!])(-n_y \partial_t \psi_2 + n_x \partial_t \psi_3) = 0.$$
(13)

3. Discrete adjoint equations

3.1. Discrete gradient calculation

The finite volume scheme of interest defines the steady-state discrete flow vector W (of size n_W) as the solution of a set of n_W non-linear equations involving W and the vector of mesh coordinates X:

$$R(W,X)=0.$$

Let us assume that the mesh is a smooth function of the vector of design parameters β (of size n_{β}), then the implicit function theorem allows to define *W* as a function of *X* and so of β [21]. Discrete gradient calculation consists of computing the derivatives of the n_f functions

$$\mathscr{J}_k(\boldsymbol{\beta}) = \mathbf{J}_k(W(\boldsymbol{\beta}), X(\boldsymbol{\beta})), \quad 1 \le k \le n_f,$$

with respect to the n_{β} design parameters. In external aerodynamic applications, n_{β} is usually much larger than n_f and the most efficient way to proceed is to use the discrete adjoint method which requires to solve n_f linear systems

$$\left(\frac{\partial R}{\partial W}\right)^T \Lambda_k = -\left(\frac{\partial J_k}{\partial W}\right)^T, \quad 1 \le k \le n_f, \tag{14}$$

and then to calculate

$$\frac{\mathrm{d}\mathscr{J}_k}{\mathrm{d}\beta} = \frac{\partial \mathrm{J}_k}{\partial X}\frac{\mathrm{d}X}{\mathrm{d}\beta} + \Lambda_k^T \left(\frac{\partial R}{\partial X}\frac{\mathrm{d}X}{\mathrm{d}\beta}\right).$$

The dominant cost is the inversion of the n_f linear systems of size n_W whereas all other classical methods solve n_β linear (or non-linear for finite-differences) systems of size n_W . The cost of solving *n* systems with the same matrix and different right-hand sides can be mitigated using specific methods like block-GMRES [50, 51] or specific CPU optimizations but in the common case where $n_f \ll n_\beta$ the adjoint method is more efficient than any direct approach.

3.2. Numerical characterization of the discrete adjoint

The adjoint vector Λ associated with one function J is usually identified with the sensitivity of J to a perturbation of the residual *R* followed by re-convergence (see [12] and references therein). Following [1, 12], we consider here a perturbation δR added to the right-hand-side of the discrete flow equations and denote by $W + \delta W$ the converged solution corresponding to the perturbed equation:

$$R(W + \delta W, X) = \delta R,$$

or at first order $\frac{\partial R}{\partial W}\delta W = \delta R$. Since $J(W + \delta W, X) \simeq J(W, X) + \frac{\partial J}{\partial W}\delta W$ the first-order change in the function of interest J due to δW is

$$\delta \mathbf{J} = \frac{\partial \mathbf{J}}{\partial W} \left(\frac{\partial R}{\partial W} \right)^{-1} \delta R,$$

or involving the adjoint vector Λ defined in (14): $\delta J = -\Lambda^T \delta R$. If only the *a*-th component of *R* at cell *m* has been altered by a small quantity δR_m^a , then the previous equation yields $\Lambda_m^a = -\delta J/\delta R_m^a$, which defines the *a*-th component of Λ at cell *m* as the limit ratio of the change in J divided by the infinitesimal change in the residual *R* at the corresponding cell and component which caused the change in flow solution and function value.

3.3. Physical characterization for 2-D Euler flows

We recall here the physical interpretation of the adjoint solution by Giles and Pierce [1]. More precisely, the discussion in [1] is based on the continuous adjoint equation and its discrete counterpart is presented here. Four physical source terms δR are defined at each individual cell: 1) local mass source at fixed stagnation pressure and total enthalpy; 2) local normal force; 3) local change in total enthalpy at fixed static and total pressure; 4) local change in total pressure at fixed total enthalpy and static pressure:

$$\delta R_m^1 = \varepsilon \begin{pmatrix} 1\\ u_x\\ u_y\\ H \end{pmatrix}, \quad \delta R_m^2 = \varepsilon \begin{pmatrix} 0\\ -\rho u_y\\ \rho u_x\\ 0 \end{pmatrix}, \quad \delta R_m^3 = \varepsilon \begin{pmatrix} -\frac{1}{2H}\\ 0\\ \frac{1}{2} \end{pmatrix}, \quad \delta R_m^4 = \varepsilon \begin{pmatrix} \frac{1}{p_0} \left(\frac{\gamma-1}{\gamma} + \frac{1}{\gamma M^2}\right)\\ \frac{u_x}{p_0} \left(\frac{\gamma-1}{\gamma} + \frac{2}{\gamma M^2}\right)\\ \frac{u_y}{p_0} \left(\frac{\gamma-1}{\gamma} + \frac{2}{\gamma M^2}\right)\\ \frac{H}{p_0} \left(\frac{\gamma-1}{\gamma} + \frac{1}{\gamma M^2}\right) \end{pmatrix}, \quad (15)$$

with $0 < \varepsilon \ll 1$ and where *H* denote the total enthalpy and *M* is the Mach number. At first order, the corresponding function variations δJ_m^1 , δJ_m^2 , δJ_m^3 , δJ_m^4 due to the source terms in cell *m*, (15), read

$$(\delta \mathbf{J}_{m}^{1}, \delta \mathbf{J}_{m}^{2}, \delta \mathbf{J}_{m}^{3}, \delta \mathbf{J}_{m}^{4}) = -(\Lambda_{m}^{1}, \Lambda_{m}^{2}, \Lambda_{m}^{3}, \Lambda_{m}^{4}) \times \begin{pmatrix} \delta R_{1,m}^{1} & \delta R_{1,m}^{2} & \delta R_{1,m}^{3} & \delta R_{1,m}^{4} \\ \delta R_{2,m}^{1} & \delta R_{2,m}^{2} & \delta R_{3,m}^{3} & \delta R_{2,m}^{4} \\ \delta R_{3,m}^{1} & \delta R_{3,m}^{2} & \delta R_{3,m}^{3} & \delta R_{4,m}^{4} \end{pmatrix},$$
(16)

where δJ_m^d corresponds to the change in J due to *d*-th change of *R* in cell *m*. Converging again the perturbed solution $W + \delta W^d$ leads to the change δJ_m^d in the function of interest. As the four changes in *R* are linearly independent, Giles and Pierce define the adjoint vector at cell *m* as the solution to (16) so, using the perturbation terms in (15), we obtain

$$(\Lambda_m^1, \Lambda_m^2, \Lambda_m^3, \Lambda_m^4) = -(\delta J_m^1, \delta J_m^2, \delta J_m^3, \delta J_m^4) \times = \frac{1}{\varepsilon} \begin{pmatrix} 1 + \frac{(\gamma - 1)}{2} M^2 & -\frac{(1 + (\gamma - 1)M^2)u_x}{\|\overline{U}\|^2} & -\frac{(1 + (\gamma - 1)M^2)u_y}{\|\overline{U}\|^2} & \frac{1 + \frac{(\gamma - 1)}{2}M^2}{H} \\ 0 & -\frac{u_y}{\rho \|\overline{U}\|^2} & \frac{u_x}{\rho \|\overline{U}\|^2} & 0 \\ -H & 0 & 0 & 1 \\ -\frac{\gamma p_0 M^2}{2} & \frac{\gamma p_0 u_x}{c^2} & \frac{\gamma p_0 u_y}{c^2} & -\frac{\gamma p_0 M^2}{2H} \end{pmatrix}.$$
(17)

The residual perturbation δR has been physically defined thus giving a physical meaning to the local discrete adjoint vector. The adjoint vector is intrinsic to the system of equations for which a similar demonstration can be done, and we can expect similar solutions from different discretizations on the same mesh.

Finally, Giles and Pierce [1] have noted for continuous adjoint that the third perturbation does not alter the pressure field for inviscid flows and hence leaves the drag and lift unchanged. From the expression of this perturbation, it is then straightforward to prove that the lift and drag continuous adjoint fields satisfy all over the fluid domain the following equation:

$$\psi_1 = H \psi_4. \tag{18}$$

This property may be compared to (5) and is seen to be well satisfied in the numerical adjoint fields (see § 5.3.1). The fourth perturbation δR^4 also preserves the static pressure at the location of the source term but the authors of [1] proved that, contrary to δR^3 , for arbitrary flow conditions, it does not preserve the static pressure field nor the streamtube structure of the base flows (in particular, the mass flux varies downstream the source term in the corresponding streamtube of the original flow).

4. Adjoint consistency of the cell-centered JST scheme

The dual consistency of the JST scheme is discussed here for 2-D FV cell-centred simulations on structured meshes. We use the classical method of equivalent differential equation which consists of introducing Taylor series expansions for all state variables and adjoint values in order to analyze the truncation error of the scheme [52, ch. 9]. Let us stress that this approach remains valid in the case of discontinuous solutions [53].

Lozano studied the adjoint consistency of the discrete adjoint of the JST scheme for both cell-centered and cell-vertex discretizations [33] of the quasi-one-dimensional compressible Euler equations. Boundary conditions using artificial dissipation (AD) were applied which lead to inconsistent discrete adjoint scheme at the boundaries. Such boundary conditions are not suitable for simulations of internal flows that require conservation and, in this work, no artificial dissipation is added to the boundary fluxes. However, several classical AD formulas may still be used for the second to last faces close to a physical boundary [54, 55]. In the following we will first consider the default discretization of our code (see equation (25) below) and then consider in §4.4 two alternative formulas (equations (26) and (27)) with different properties with respect to dual consistency. Finally, this analysis is completed in § 5.2 to 5.4 by numerical and visual examination of the residuals of the continuous adjoint equation calculated for the discrete lift and drag adjoint fields.

The reference continuous equations will be the adjoint of Euler equations in transformed coordinates. Jameson presented these equations in 2-D and 3-D [4]. Later on, Giles and Pierce derived the corresponding direct differentiation equation in 2-D [56]. In this framework, the physical space (typically about an airfoil) is seen as the image of the unit domain $[0,1] \times [0,1]$ with coordinates (ξ, η) . The transformed 2-D Euler equations in the (ξ, η) -coordinates are well-known and, for functions of the form (1), the adjoint equations read

$$-\frac{\partial\Lambda^{T}}{\partial\xi}\left(\frac{\partial y}{\partial\eta}A(W) - \frac{\partial x}{\partial\eta}B(W)\right) - \frac{\partial\Lambda^{T}}{\partial\eta}\left(-A(W)\frac{\partial y}{\partial\xi} + B(W)\frac{\partial x}{\partial\xi}\right) = 0,$$
(19)

where A(w) and B(w) are the Jacobians of Euler flux in the physical x and y directions. Let us assume that the wall corresponds to the $\xi = 0$ boundary and that the function of interest is the force applied by the fluid on the solid in

direction $\overline{d} = (d_x, d_y)$, then the corresponding boundary condition reads:

$$-\Lambda^T \left(A(W) \frac{\partial y}{\partial \eta} - B(W) \frac{\partial x}{\partial \eta} \right) - \left(\frac{\partial y}{\partial \eta} d_x - \frac{\partial x}{\partial \eta} d_y \right) \frac{\partial p}{\partial W} = 0 \quad \text{at} \ \xi = 0.$$

It can be simplified by benefiting from the specific form of the Jacobian at a wall yielding

$$\Lambda_2 \frac{\partial y}{\partial \eta} - \Lambda_3 \frac{\partial x}{\partial \eta} + \left(\frac{\partial y}{\partial \eta} d_x - \frac{\partial x}{\partial \eta} d_y\right) = 0.$$
⁽²⁰⁾

The adjoint consistency of the FV scheme of interest is discussed hereafter referring to the formal equations (19) and (20). Using a structured mesh, the JST scheme in the *i*-direction reads (the *j* subscripts have been dropped for the sake of readability):

$$F_{i+1/2}^{JST} = \frac{1}{2} (\mathbf{F}(W_i) + \mathbf{F}(W_{i+1})) \cdot S_{i+1/2} - k^2 v_{i+1/2} \kappa_{i+1/2} (W_{i+1} - W_i) + \overline{k^4}_{i+1/2} \kappa_{i+1/2} (W_{i+2} - 3W_{i+1} + 3W_i - W_{i-1})$$
(21)

$$=\frac{|p_{i+1}-2p_i+p_{i-1}|}{(p_{i+1}+2p_i+p_{i-1})} \qquad \qquad \mathbf{v}_{i+1/2}=\max(\mathbf{v}_i,\mathbf{v}_{i+1}) \tag{22}$$

$$\overline{k^4}_{i+1/2} = \max(0, k^4 - v_{i+1/2}k^2) \qquad \qquad \kappa_{i+1/2} = |\overline{U}_{i+1/2}.S_{i+1/2}| + c_{i+1/2} ||S_{i+1/2}||, \tag{23}$$

where $\mathbf{F} = (F_x, F_y)$. The fluid velocity \overline{U} and the speed of sound *c* at the interface i + 1/2 are evaluated from one of the classical conserved variable means. Dual consistency close to the boundary depends on the specific flux formulas at the boundary and second to last interfaces:

$$F_{1/2}^{JST} = \mathbf{F}(W_b) \cdot S_{1/2}$$
 (24)

$$F_{3/2}^{JST_a} = \frac{1}{2} (\mathbf{F}(W_1) + \mathbf{F}(W_2)) \cdot S_{3/2} - k^2 v_{3/2} \kappa_{3/2} (W_2 - W_1) + \overline{k^4}_{3/2} \kappa_{3/2} (W_3 - 3W_2 + 2W_1)$$
(25)

where $p_0 = 2p_b - p_1$ is used in the evaluation of v_1 , and W_b is a boundary state satisfying all Dirichlet-like boundary conditions. For the sake of comparison, two alternative formulas [54, 55] will be considered:

$$F_{3/2}^{JST_b} = \frac{1}{2} (\mathbf{F}(W_1) + \mathbf{F}(W_2)) \cdot S_{3/2} - k^2 v_{3/2} \kappa_{3/2} (W_2 - W_1) + \overline{k^4}_{3/2} \kappa_{3/2} (W_3 - 2W_2 + W_1),$$
(26)

$$F_{3/2}^{JST_c} = \frac{1}{2} (\mathbf{F}(W_1) + \mathbf{F}(W_2)) \cdot S_{3/2} - k^2 v_{3/2} \kappa_{3/2} (W_2 - W_1) + \overline{k^4}_{3/2} \kappa_{3/2} (W_3 - 3W_2 + 3W_1 - W_g), \quad (27)$$

where W_g is a mirror state of W_1 w.r.t. the boundary.

Note that at specific faces where either $\overline{U} \cdot S = 0$, or $k^4 - vk^2 = 0$, or $v_i = v_{i+1}$, the flux is not differentiable. This issue is discussed in [57] for a simulation about a symmetric airfoil, with a symmetric mesh and zero angle of attack leading to two complete lines of faces where $|\overline{U} \cdot S|$ is extremely close to machine-level-zero. The small irregularities of adjoint quantities that appear close to these lines are cured by regularization but no such problem is observed for more complex cases and, most generally, this question is discarded [58] considering that the occurrence of such equalities is marginal in practice.

Under the classical assumption that $\Delta\xi$ and $\Delta\eta$ vary smoothly and have the same order of magnitude, the consistency of the discrete adjoint of equations (21) to (24) completed by (25), (26) or (27), is studied. The main result of this section is the following.

Lemma 1. For a wall integral, the discrete discrete adjoint of the finite-volume JST scheme is:

- consistent with the continuous adjoint equations (19) in interior cells;
- consistent with the continuous adjoint equations (19) in a penultimate cell w.r.t. a boundary using $F_{3/2}^{JST_b}$ whereas it is inconsistent using $F_{3/2}^{JST_a}$ or $F_{3/2}^{JST_c}$;
- consistent with the wall boundary condition (20) in a cell adjacent to a wall.

The first and third results are independent of the choice of the $F_{3/2}^{JST}$ formula.

Unfortunately, the choice of $F_{3/2}^{JST_b}$ induces significant robustness issues in the simulations on very fine meshes and we finally discuss in §4.5 how to slightly alter the exact Jacobian obtained with $F_{3/2}^{JST_a}$ and $F_{3/2}^{JST_c}$ to get adjoint consistency.

4.1. Consistency of discrete adjoint inside the domain

The discrete adjoint equation at a current cell (i, j) reads

$$(\Lambda_{(i-2,j)}^{T} - \Lambda_{(i-1,j)}^{T}) \frac{\partial F_{i-3/2,j}}{\partial W_{(i,j)}} + (\Lambda_{(i-1,j)}^{T} - \Lambda_{(i,j)}^{T}) \frac{\partial F_{i-1/2,j}}{\partial W_{(i,j)}}$$
(28)

$$+(\Lambda_{(i,j)}^{T} - \Lambda_{(i+1,j)}^{T})\frac{\partial F_{i+1/2,j}}{\partial W_{(i,j)}} + (\Lambda_{(i+1,j)}^{T} - \Lambda_{(i+2,j)}^{T})\frac{\partial F_{i+3/2,j}}{\partial W_{(i,j)}}$$
(29)

$$+(\Lambda_{(i,j-2)}^{T}-\Lambda_{(i,j-1)}^{T})\frac{\partial F_{i,j-3/2}}{\partial W_{(i,j)}}+(\Lambda_{(i,j-1)}^{T}-\Lambda_{(i,j)}^{T})\frac{\partial F_{i,j-1/2}}{\partial W_{(i,j)}}$$
(30)

$$+(\Lambda_{(i,j)}^{T}-\Lambda_{(i,j+1)}^{T})\frac{\partial F_{i,j+1/2}}{\partial W_{(i,j)}}+(\Lambda_{(i,j+1)}^{T}-\Lambda_{(i,j+2)}^{T})\frac{\partial F_{i,j+3/2}}{\partial W_{(i,j)}} = 0.$$
(31)

Only fluxes in the *i*-direction appear in (28)-(29), while only fluxes in the *j*-direction appear in (30)-(31) and we will analyze them separately. This is done below in the *i*-direction (again dropping the *j* subscripts). The contribution of the centered flux in (28)-(29) is

$$\frac{1}{2} \left(\left(\Lambda_{i-1}^T - \Lambda_i^T \right) \frac{\partial \mathbf{F}}{\partial W_i} S_{i-1/2} + \left(\Lambda_i^T - \Lambda_{i+1}^T \right) \frac{\partial \mathbf{F}}{\partial W_i} S_{i+1/2} \right).$$
(32)

The *i* and *j* subscripts and ξ and η coordinates are linked by the simple affine transformations

$$\xi(i) = \frac{i-1}{i_{max}-1} = (i-1)\Delta\xi, \qquad \eta(j) = \frac{j-1}{j_{max}-1} = (j-1)\Delta\eta,$$

and the expression of the surface vectors is easily derived from those of the coordinates

$$S_{i+1/2,j} = \begin{pmatrix} y(\xi(i+1/2), \eta(j+1/2)) - y(\xi(i+1/2), \eta(j-1/2)) \\ -x(\xi(i+1/2), \eta(j+1/2)) + x(\xi(i+1/2), \eta(j-1/2)) \end{pmatrix}$$

The two terms in (32) are hence consistent with

$$-\frac{1}{2}\frac{\partial\Lambda^{T}}{\partial\xi}\left(\frac{\partial y}{\partial\eta}A-\frac{\partial x}{\partial\eta}B\right)\Delta\xi\Delta\eta$$

respectively at points (i - 1/2, j) and (i + 1/2, j), with $\Delta \xi \Delta \eta$ the volume of a cell, and the sum of both contributions is a consistent approximation of

$$-\frac{\partial \Lambda^T}{\partial \xi} \left(\frac{\partial y}{\partial \eta} A - \frac{\partial x}{\partial \xi} B \right) \Delta \xi \Delta \eta$$

at point (i, j). Moreover it is second-order accurate as it uses symmetric means and differences w.r.t. $(\xi(i), \eta(j))$. Carrying out the corresponding expansions for the linearized fluxes in the *j*-direction, the second term of equation (19) times $\Delta\xi\Delta\eta$ is recovered. The first part of the discrete adjoint equation, obtained by isolating the differentiation of the centered flux, is hence a consistent discretization of equation (19) up to a multiplicative $\Delta\xi\Delta\eta$ factor.

After this first step, the discussion of the interior cells adjoint consistency of the JST scheme comes back to the examination of all the other terms in (28)-(31) and the question whether other second-order terms in $\Delta\xi$ and $\Delta\eta$ appear

(inconsistency) or only higher-order terms appear (consistency). The terms in (28)-(29) that involve the derivatives of the sensor, read

$$k^{2} \bigg(\left(\Lambda_{i-2}^{T} - \Lambda_{i-1}^{T} \right) \frac{\partial v_{i-3/2}}{\partial W_{(i,j)}} \kappa_{i-3/2} \bigg(- \left(W_{i-2} - W_{i-1} \right) - 1_{[\overline{k^{4}}_{i-3/2} > 0]} (W_{i} - 3W_{i-1} + 3W_{i-2} - W_{i-3}) \bigg) \\ + \left(\Lambda_{i-1}^{T} - \Lambda_{i}^{T} \right) \frac{\partial v_{i-1/2}}{\partial W_{(i,j)}} \kappa_{i-1/2} \bigg(- \left(W_{i-1} - W_{i} \right) - 1_{[\overline{k^{4}}_{i-1/2} > 0]} (W_{i+1} - 3W_{i} + 3W_{i-1} - W_{i-2}) \bigg) \\ + \left(\Lambda_{i}^{T} - \Lambda_{i+1}^{T} \right) \frac{\partial v_{i+1/2}}{\partial W_{(i,j)}} \kappa_{i+1/2} \bigg(- \left(W_{i} - W_{i+1} \right) - 1_{[\overline{k^{4}}_{i+1/2} > 0]} (W_{i+2} - 3W_{i+1} + 3W_{i} - W_{i-1}) \bigg) \\ + \left(\Lambda_{i+1}^{T} - \Lambda_{i+2}^{T} \right) \frac{\partial v_{i+3/2}}{\partial W_{(i,j)}} \kappa_{i+3/2} \bigg(- \left(W_{i+1} - W_{i+2} \right) - 1_{[\overline{k^{4}}_{i+3/2} > 0]} (W_{i+3} - 3W_{i+2} + 3W_{i+1} - W_{i}) \bigg) \bigg),$$
(33)

where $1_{[\overline{k^4}_{i+1/2}>0]}$ stands for 1 if $\overline{k^4}_{i+1/2}$ is strictly positive and 0 if not. As the spectral radius κ is $O(\Delta \eta)$, all the terms in (33) are at least $O(\Delta \xi^2 \Delta \eta)$. The terms of (28)-(29) that involve the derivatives of the spectral radius are

$$(\Lambda_{i-1}^{T} - \Lambda_{i}^{T}) \frac{\partial \kappa_{i-1/2}}{\partial W_{(i,j)}} \Big(-k^{2} \nu_{i-1/2} (W_{i-1} - W_{i}) + \overline{k^{4}}_{i-1/2} (W_{i+1} - 3W_{i} + 3W_{i-1} - W_{i-2}) \Big) \\ (\Lambda_{i}^{T} - \Lambda_{i+1}^{T}) \frac{\partial \kappa_{i+1/2}}{\partial W_{(i,j)}} \Big(-k^{2} \nu_{i+1/2} (W_{i} - W_{i+1}) + \overline{k^{4}}_{i+1/2} (W_{i+1} - 3W_{i} + 3W_{i} - W_{i-1}) \Big).$$
(34)

As κ and its derivatives w.r.t. W are $O(\Delta \eta)$ and as v is $O(\Delta \xi^2)$ these terms are $O(\Delta \xi^4 \Delta \eta)$. The terms arising when differentiating the first-difference and the third-difference are

$$(\Lambda_{i-2}^{T} - \Lambda_{i-1}^{T})(\kappa_{i-3/2} \overline{k^{4}}_{i-3/2}) + (\Lambda_{i-1}^{T} - \Lambda_{i}^{T})(-k^{2} \nu_{i-1/2} \kappa_{i-1/2} - 3 \overline{k^{4}}_{i-1/2} \kappa_{i-1/2}) \\ + (\Lambda_{i}^{T} - \Lambda_{i+1}^{T})(k^{2} \nu_{i+1/2} \kappa_{i+1/2} + 3 \overline{k^{4}}_{i+1/2} \kappa_{i+1/2}) + (\Lambda_{i+1}^{T} - \Lambda_{i+2}^{T})(-\kappa_{i+3/2} \overline{k^{4}}_{i+3/2})$$

and may be rewritten as

$$\begin{aligned} & (\Lambda_{i-2}^T - \Lambda_{i-1}^T) \kappa_{i-3/2} \, \overline{k^4}_{i-3/2} - 3(\Lambda_{i-1}^T - \Lambda_i^T) \kappa_{i-1/2} \, \overline{k^4}_{i-1/2} \\ &+ 3(\Lambda_i^T - \Lambda_{i+1}^T) \kappa_{i+1/2} \, \overline{k^4}_{i+1/2} - (\Lambda_{i+1}^T - \Lambda_{i-2}^T) \kappa_{i+3/2} \, \overline{k^4}_{i+3/2} \\ &- k^2 ((\Lambda_{i-1}^T - \Lambda_i^T) \mathbf{v}_{i-1/2} \, \kappa_{i-1/2} - (\Lambda_i^T - \Lambda_{i+1}^T) \mathbf{v}_{i+1/2} \, \kappa_{i+1/2}). \end{aligned}$$

The last two terms that stem from first-difference dissipation fluxes, are both $O(\Delta\xi^3\Delta\eta)$ as the sensor in ξ (*I*-mesh) direction is $O(\Delta\xi^2)$. The possibly problematic terms are the four first terms stemming from the third-difference dissipation fluxes. These are individually $O(\Delta\xi\Delta\eta)$ terms and the question is whether their linear combination is a higher-order term. If the algebraic expression of $\overline{k^4}$ as function of the state variables is the same for all four values, then a third-order difference is identified and linear combination of these four terms is $O(\Delta\xi^4\Delta\eta)$. If some of the $v_{l+1/2}$ are equal to the left value v_l and some to the right value v_{l+1} but none of the $\overline{k^4}$ is zero, the terms stemming from the differentiation of third-order differences may be rewritten as

$$\begin{split} &(\Lambda_{i-2}^{T} - \Lambda_{i-1}^{T})\kappa_{i-3/2} k^{4} - 3(\Lambda_{i-1}^{T} - \Lambda_{i}^{T})\kappa_{i-1/2} k^{4} + 3(\Lambda_{i}^{T} - \Lambda_{i+1}^{T})\kappa_{i+1/2} k^{4} - (\Lambda_{i+1}^{T} - \Lambda_{i+2}^{T})\kappa_{i+3/2} k^{4} \\ &- (\Lambda_{i-2}^{T} - \Lambda_{i-1}^{T})\kappa_{i-3/2} k^{2} \mathbf{v}_{i-3/2} + 3(\Lambda_{i-1}^{T} - \Lambda_{i}^{T})\kappa_{i-1/2} k^{2} \mathbf{v}_{i-1/2} \\ &- 3(\Lambda_{i}^{T} - \Lambda_{i+1}^{T})\kappa_{i+1/2} k^{2} \mathbf{v}_{i+1/2} + (\Lambda_{i+1}^{T} - \Lambda_{i+2}^{T})\kappa_{i+3/2} k^{2} \mathbf{v}_{i+3/2}. \end{split}$$

In this case, the sum of the terms involving k^4 is $O(\Delta\xi^4\Delta\eta)$ and the terms in k^2 may be individually identified as $O(\Delta\xi^3\Delta\eta)$ terms. For inconsistency to be observed, it is hence necessary that: (a) due to the max function in equation (22), the actual formulas of the involved $\overline{k^4}$ are not the same up to a shift of subscripts; (b) some of the $\overline{k^4}$ are zero. (Note that these conditions are expected to appear at a marginal number of cells in particular as v is very close to zero

except in the vicinity of shock waves. Also note that these conditions are not even sufficient for dual inconsistency $-if \overline{k^4}_{i-3/2} = \overline{k^4}_{i+3/2} = 0$ and $\overline{k^4}_{i+1/2} \neq 0$, $\overline{k^4}_{i+3/2} \neq 0$ or crisscross, dual consistency is observed). Such conditions for inconsistency thus correspond to local non-differentiability of the JST scheme. This may be compared with the results of reference [34] and the local lack of dual consistency of the studied schemes where upwinding changes.

4.2. Consistency of the discrete adjoint at a penultimate cell w.r.t. a boundary

In a penultimate cell of indices (2, j), the previous equations are slightly altered as numerical fluxes $F_{1/2,j}$ and $F_{3/2,j}$ have specific definitions involving a boundary state, $W_{b_{1/2,j}}$. Actually $W_{b_{1/2,j}}$ depends on the adjacent conservative variables $W_{1,j}$ and the $S_{1/2,j}$ surface vector only; W_b satisfies all Dirichlet like relations to be imposed at the boundary. The numerical flux at the i=1/2 boundary interface is given by (24). The numerical flux at the i=3/2 boundary interface is assumed in this subsection to be defined by (25). This formula is satisfactory from a robustness point of view but it induces an inconsistent scheme in the last two cells adjacent to a boundary. This issue will be fixed by using formulas (26) and (27) in §4.4¹.

We now consider the discrete adjoint equation in the penultimate cell (2, j) (see Fig. 1). Note first that the contributions of the centered flux are standard for both mesh directions since $F_{1/2,j}^{JST}$ does not depend on $W_{2,j}$. The terms of lines (30)-(31) are the same as in a current cell and do not need to be investigated again. Those of lines (28)-(29) read

$$(\Lambda_1^T - \Lambda_2^T)\frac{\partial F_{3/2}}{\partial W_2} + (\Lambda_2^T - \Lambda_3^T)\frac{\partial F_{5/2}}{\partial W_2} + (\Lambda_3^T - \Lambda_4^T)\frac{\partial F_{7/2}}{\partial W_2} = 0$$
(35)

(dropping *j* indices) as $F_{1/2}$ does not depend on W_2 . The current face contributions stemming from the differentiation of the sensor and the spectral radius have been bounded individually in the previous subsection. We hence only need to look at the specific contributions of the 3/2 face that depends on the boundary condition through v_1 in $v_{3/2}$. Differentiating the sensor yields

$$k^{2}(\Lambda_{1}^{T}-\Lambda_{2}^{T})\frac{\partial v_{3/2}}{\partial W_{2}}\kappa_{3/2}\Big(-(W_{2}-W_{1})-1_{[\overline{k^{4}}_{3/2}>0]}(W_{3}-3W_{2}+2W_{1})\Big)$$

that is $O(\Delta\xi^2\Delta\eta)$. When differentiating the spectral radius, the only specific term depending on the boundary condition, is also the one stemming from $F_{3/2}^{JST}$,

$$(\Lambda_1^T - \Lambda_2^T) \frac{\partial \kappa_{3/2}}{\partial W_2} \Big(-k^2 v_{3/2} (W_2 - W_1) + \overline{k^4}_{3/2} (W_3 - 3W_2 + 2W_1) \Big).$$

The first part of this expression is $O(\Delta\xi^3\Delta\eta)$ (a more precise assertion depends whether $v_{3/2} = v_1$ that is $O(\Delta\xi)$ or $v_{3/2} = v_2$ that is $O(\Delta\xi^2)$). The second part of this expression is $O(\Delta\xi^2\Delta\eta)$. None of them hence prevents dual consistency. Finally, the terms arising from the differentiation of the differences terms in (35) read

$$(\Lambda_1^T - \Lambda_2^T)(-k^2 \nu_{3/2} \kappa_{3/2} - 3\overline{k^4}_{3/2} \kappa_{3/2}) + (\Lambda_2^T - \Lambda_3^T)(k^2 \nu_{5/2} \kappa_{5/2} + 3\overline{k^4}_{5/2} \kappa_{5/2}) + (\Lambda_3^T - \Lambda_4^T)(-\kappa_{7/2} \overline{k^4}_{7/2}).$$

They may be rewritten as

$$-3(\Lambda_{1}^{T} - \Lambda_{2}^{T})\overline{k^{4}}_{3/2}\kappa_{3/2} + 3(\Lambda_{2}^{T} - \Lambda_{3}^{T})\overline{k^{4}}_{5/2}\kappa_{5/2} - (\Lambda_{3}^{T} - \Lambda_{4}^{T})\kappa_{7/2} \overline{k^{4}}_{7/2}$$

$$-(\Lambda_{1}^{T} - \Lambda_{2}^{T})k^{2}\nu_{3/2} \kappa_{3/2} + (\Lambda_{2}^{T} - \Lambda_{3}^{T})k^{2}\nu_{5/2} \kappa_{5/2}.$$

$$(36)$$

The two terms of the last line are at least $O(\Delta\xi^2\Delta\eta)$ (a more precise assertion depends whether $v_{3/2}$ is equal to v_1 or v_2). The sum of the terms of the first line is only $O(\Delta\xi\Delta\eta)$ and introduces an inconsistency. (Compared to the current-point equation, due to the specific $F_{1/2,j}$ formula, a $(\Lambda_0^T - \Lambda_1^T)\overline{k^4}_{1/2}\kappa_{1/2}$ is missing to have a third-order difference to appear.)

difference to appear.) Whether $F_{3/2}^{JST_b}$ or $F_{3/2}^{JST_c}$ leads to a dual-consistent scheme is discussed in § 4.4. How the exact linearization of $F_{3/2}^{JST_a}$ (and also $F_{3/2}^{JST_c}$) can be slightly modified to obtain dual consistency is discussed in § 4.5.

¹As the factors multiplying $\overline{k_{3/2}^4} \kappa_{3/2}$ in (25) (26) and (27) are respectively first-, second-, and third-order terms, this is the simplest way to discuss dual consistency for these three $F_{3/2}^{JST}$ formulas.

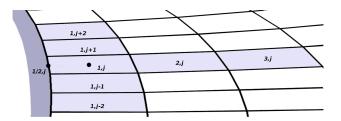


Figure 1: Location of the state variable W and the corresponding boundary variable W_b for the (1, j) cell. Stencil of the JST scheme for this cell.

4.3. Consistency of discrete adjoint at a wall boundary cell

The discrete counterpart of the output functional (1) reads

$$J = \sum_{j} p(W_{b_{(1/2,j)}}) S_{(1/2,j)}.\overline{d},$$
(37)

where (1/2, j) are the wall indices. We stress that the static pressure *p* is evaluated for the boundary state W_b that also appears in the boundary flux (24). The discrete adjoint equation in a cell adjacent to a wall-boundary (see cell (1, j) in Fig. 1) then reads

$$\sum_{k} \Lambda_{k}^{T} \frac{\partial R_{k}}{\partial W_{(1,j)}} = -\frac{\partial J}{\partial W_{b_{(1/2,j)}}} \frac{\partial W_{b_{(1/2,j)}}}{\partial W_{(1,j)}}.$$
(38)

Due to the stencil of the JST scheme in (21), (25) and (24), the k subscript varies in $\{(1, j-2), (1, j-1), (1, j), (1, j+1), (1, j+2), (2, j), (3, j)\}$ as illustrated in Fig. 1. The expanded expression of (38) reads

$$(\Lambda_{(1,j-2)}^{T} - \Lambda_{(1,j-1)}^{T}) \frac{\partial F_{1,j-3/2}}{\partial W_{(1,j)}} + (\Lambda_{(1,j-1)}^{T} - \Lambda_{(1,j)}^{T}) \frac{\partial F_{1,j-1/2}}{\partial W_{(1,j)}}$$
(39)

$$+(\Lambda_{(1,j)}^{T}-\Lambda_{(1,j+1)}^{T})\frac{\partial F_{1,j+1/2}}{\partial W_{(1,j)}}+(\Lambda_{(1,j+1)}^{T}-\Lambda_{(1,j+2)}^{T})\frac{\partial F_{1,j+3/2}}{\partial W_{(1,j)}}$$
(40)

$$+(\Lambda_{(2,j)}^{T}-\Lambda_{(3,j)}^{T})\frac{\partial F_{5/2,j}}{\partial W_{(1,j)}}+(\Lambda_{(1,j)}^{T}-\Lambda_{(2,j)}^{T})\frac{\partial F_{3/2,j}}{\partial W_{(1,j)}}$$
(41)

$$-\Lambda_{(1,j)}^T \frac{\partial F_{1/2,j}}{\partial W_{(j,1)}} = -\frac{\partial J}{\partial W_{b_{(i,1/2)}}} \frac{\partial W_{b_{(i,1/2)}}}{\partial W_{(1,j)}}.$$
(42)

As noted by Nadarajah et al. [27], this equation mixes $O(\Delta \eta)$ terms (in (42) only) and higher order terms (in all three first lines), and as the mesh is refined the continuous adjoint wall boundary condition is recovered from the first-order terms. Keeping only the $O(\Delta \eta)$ terms, the previous equations yield

$$-\Lambda_{(i,1)}^{T} \begin{pmatrix} 0\\ Sx_{(1/2,j)}\\ Sy_{(1/2,j)}\\ 0 \end{pmatrix} \frac{\partial p_{b_{(1/2,j)}}}{\partial W_{b_{(1/2,j)}}} \frac{\partial W_{b_{(1/2,j)}}}{\partial W_{(1,j)}} \simeq -\frac{\partial((-\overline{S_{(1/2,j)}} \cdot \overline{d})p_{b_{(1/2,j)}})}{\partial W_{b_{(1/2,j)}}} \frac{\partial W_{b_{(1/2,j)}}}{\partial W_{(1,j)}},$$

which may be simplified into

$$\Lambda_{(i,1)}^2 Sx_{(1/2,j)} + \Lambda_{(i,1)}^3 Sy_{(1/2,j)} \simeq -\overline{S_{(1/2,j)}} \cdot \overline{d}.$$
(43)

Note that it involves metric terms at the wall and the adjoint at adjacent cells and also that it has been derived by equalizing lower-order (i.e., first-order) terms in space. How accurately equation (43) is satisfied is discussed in sections 5.2 to 5.4.

4.4. Alternative $F_{3/2}$ formulas $F_{3/2}^{JST_b}$ and $F_{3/2}^{JST_c}$ and adjoint consistency

The discrete adjoint of the cell-centered JST scheme (21) to (25) is thus adjoint-consistent except at penultimate cells w.r.t. a boundary. Possible changes in $F_{3/2}$ to get adjoint consistency are discussed here in relation with classical publications [54, 55] that presented specific formulas for JST AD close to the boundaries of a structured mesh for steady state flow simulations.

A satisfactory modification of $F_{3/2}^{JST}$ for dual consistency, would substitute

$$F_{3/2}^{JST_b} = \frac{1}{2} (\mathbf{F}(W_1) + \mathbf{F}(W_2)) \cdot S_{3/2} - k^2 \mathbf{v}_{3/2} \mathbf{\kappa}_{3/2} (W_2 - W_1) + \overline{k^4}_{3/2} \mathbf{\kappa}_{3/2} (W_3 - 2W_2 + W_1)$$

to $F_{3/2}^{JST_a}$. To check this, first note that $(W_3 - 2W_2 + W_1)$ in (26) is a second-order difference whereas $(W_3 - 3W_2 + 2W_1)$ in (25) is a first-order term. Consequently, the terms of $(\partial F_{3/2}/\partial W_1)$ and $(\partial F_{3/2}/\partial W_2)$ stemming from the differentiation of the spectral radius or the sensor may not be of lower order than their counterpart in the calculations of §4.1 to §4.3. When differentiating the $(W_3 - 2W_2 + W_1)$ factor, the contribution in $(\partial F_{3/2}/\partial W_3)$ is unchanged; the contribution in $(\partial F_{3/2}/\partial W_2)$ precisely cures the issue that appears in line (36); the contribution in $(\partial F_{3/2}/\partial W_1)$ is a $O(\Delta\xi\Delta\eta)$ term in line (41) dominated by the $O(\Delta\eta)$ terms of line (42).

Moreover, this $(W_3 - 2W_2 + W_1)$ factor is one of the adapted discretizations of the third-order difference that is recommended close to boundaries in [54, B1 formula] and [55]. Compared to the corresponding factor in (25), it doesn't introduce inconsistent terms in the discretization of the Euler equations in the last two rows of cells close to a physical boundary.

The numerical flux (26) has been implemented and proved to be more accurate than (25). For example, for our 2-D subsonic test case (§5.4), using $F_{3/2}^{JST_b}$, the spurious drag values calculated on a hierarchy of embedded meshes are 30.1, 8.7, 3.2 and 1.8 drag counts on the 128², 256², 512² and 1024²-cell meshes, to be compared to 37.9, 11.3, 4.0 and 2.1 drag counts using $F_{3/2}^{JST_a}$. Besides, other accuracy indicators like total enthalpy losses also support the superiority of $F_{3/2}^{JST_b}$ over $F_{3/2}^{JST_a}$.

This discretization, unfortunately, significantly reduces the robustness of the JST scheme on very fine meshes and, when selecting it, we could not get converged flows for our transonic (§5.3) and subsonic (§5.4) 2-D test cases and our finest meshes (with 2048² and 4096² cells). As there is no artificial dissipation in $F_{1/2}$, the $\overline{k^4}_{3/2}\kappa_{3/2}(W_3 - 2W_2 + W_1)$ term of this $F_{3/2}$ flux introduces an anti-dissipative term in the equivalent equation of the cells adjacent to the boundary. Most probably, this is the reason of this loss of robustness.

Once again, formulas involving AD at boundaries are not taken into consideration here in order to keep the same discretizations for internal and external flows. On the contrary, regarding the second to last faces, formulas recommended by Swanson and Turkel in [55] are recalled and studied with respect to the inconsistency issue that appeared in §4.2. W_g being a mirror state of W_1 w.r.t. the boundary, the final formula they recommend reads

$$F_{3/2}^{JST_c} = \frac{1}{2} (\mathbf{F}(W_1) + \mathbf{F}(W_2)) \cdot S_{3/2} - k^2 v_{3/2} \kappa_{3/2} (W_2 - W_1) + \overline{k^4}_{3/2} \kappa_{3/2} (W_3 - 3W_2 + 3W_1 - W_g).$$

It is simply a standard discretization leading to a standard fourth-order dissipative term in the penultimate cells w.r.t. to the boundary [55, Eq. (2.17)]. This formula is one of those available in our code [59] with $W_g = 2Wb - W_1$. Let us note first that $(W_3 - 3W_2 + 3W_1 - W_g)$ is a third-order term in space as for formula $F_{3/2}^{JST_b}$. The same arguments as above are relevant and the adjoint (in)consistency discussion in cell (2, j) is again reduced to the examination of the terms stemming from the differentiation of the $(W_3 - 3W_2 + 3W_1 - W_g)$ factor in $(\partial F_{3/2}/\partial W_3)$, $(\partial F_{3/2}/\partial W_2)$, $(\partial F_{3/2}/\partial W_1)$ compared to those of the default discretization. As in the discussion just above, $(\partial F_{3/2}/\partial W_3)$ is unchanged and $(\partial F_{3/2}/\partial W_1)$ brings $O(\Delta\xi\Delta\eta)$ terms in line (41) that are dominated by the $O(\Delta\eta)$ terms of line (42). Finally $(\partial F_{3/2}/\partial W_2)$ contribution in (36) is a $-3(\Lambda_1^T - \Lambda_2^T)\overline{k^4}_{3/2}\kappa_{3/2}$ term just as in the default $F_{3/2}^{JST_a}$ discretization and inconsistency is also noticed for the penultimate cells w.r.t. a boundary.

4.5. Modified linearization of $F_{3/2}^{JST_a}$ and $F_{3/2}^{JST_c}$ for adjoint consistency

Adjoint consistency may be recovered with a minor and local approximation in the Jacobian of the scheme. Following the analysis of § 4.2, the needed change in the differentiation of the $F_{3/2,j}^{JST_a}$ flux is the replacement of

$$-3(\Lambda_{1}^{T}-\Lambda_{2}^{T})\overline{k^{4}}_{3/2}\kappa_{3/2} \quad \text{by} \quad -2(\Lambda_{1}^{T}-\Lambda_{2}^{T})\overline{k^{4}}_{3/2}\kappa_{3/2} \quad \text{in} \quad (\partial F_{3/2,j}/\partial W_{2}),$$

when differentiating the third-order difference. The same modification in the linearization of $F_{3/2,j}^{JST_c}$ is required to ensure dual consistency as shown in § 4.4.

Whereas it was simpler to start the dual consistency analysis for $F_{3/2}^{JST_a}$ and then adapt it for $F_{3/2}^{JST_b}$ and $F_{3/2}^{JST_c}$, only $F_{3/2}^{JST_c}$ is considered from now on. The robustness of the numerical simulations and the final level of the steady state residuals on very fine meshes are almost as satisfactory as with $F_{3/2}^{JST_a}$. Besides, $F_{3/2}^{JST_c}$ does not introduce any inconsistency or reduction of the order of accuracy for the cells adjacent to the boundaries and their first neighbors. Concerning the adjoint fields, the modified linearization is used when discussing adjoint consistency; the exact linearization and possibly also the modified one are used in the other sections.

These linearizations are compared by using the energy component of the lift adjoint in Fig. 2. The dual inconsistency is illustrated by spurious oscillations in the iso-lines in the vicinity of the two problematic cells. The amplitude of these oscillations is damped away from the wall and is reduced when using finer meshes. As expected, the oscillations vanish when the consistent adjoint linearization is used.

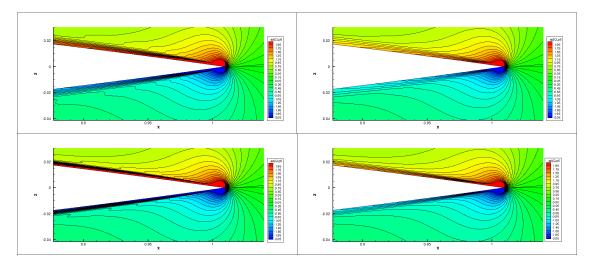


Figure 2: $(M_{\infty} = 0.4, \alpha = 5^{\circ})$ Energy component of the lift adjoint. Top 2049×2049 mesh, bottom 4097×4097 mesh – Left, inconsistent discrete adjoint, right consistent discrete adjoint.

5. Numerical experiments

We present here the discrete direct and adjoint solutions to inviscid flows around the NACA0012 airfoil in different regimes. Steady-state solutions are computed with the *elsA* code [59] on a series of six structured meshes ranging from 129×129 to 4097×4097 nodes used and described in [60]. The far field boundary is set at about 150 chords. The computations have been converged with a second-order accurate FV method using the JST scheme (21)-(24) and (27) with $k^2 = 0.5$ and $k^4 = 0.032$, except for the subsonic flow for which we used $k^2 = 0$ and $k^4 = 0.032$. The derivatives of the lift and the drag w.r.t. the flow field variables in the discrete adjoint equation (14) were calculated by using the post-processing tool from [61] before the adjoint equations were solved by the adjoint module of *elsA* [62?] for the two functions and the complete set of meshes.

5.1. Main results

Summary 1. The dual consistency of the linearization of the JST scheme (21) to (24) and (27), involving the minor correction of $dF_{3/2}^{JST_c}$ introduced in § 4.2, is confirmed by discretizing the continuous adjoint equations for consistent and inconsistent discrete adjoint fields on a hierarchy of grids and computing the corresponding residuals. The residuals highlight two types of zones were their norm keeps large values as the mesh is refined: (i) zones of discontinuity of the adjoint field; (ii) zones of numerical divergence of the adjoint field. In both types of location, a Taylor expansion cannot be applied and dual consistency is not discussed.

Among the zones where numerical divergence is observed and mathematical divergence is suspected (see below) we focus on the vicinity of the wall and the stagnation streamline: in the framework of the physical source terms approach [1], it appears that the fourth source term δR^4 in (15) is the one responsible for the numerical divergence at the wall. The way it disturbs the flow is described. The numerical divergence of the adjoint components in the vicinity of the wall and stagnation streamline appears to be numerically more complex than the algebraic law derived in [1] under simplifying assumptions.

Completing the dual consistency discussions, complementary analysis is provided in the case of the supersonic flow providing insight on the structure of the theoretical continuous adjoint field. Finally, the jump relations on the adjoint derivatives derived in § 2.2 are numerically checked on the finest grid.

Let us stress, first, that an adjoint discontinuity is typically observed at the trailing edge of a supersonic flow. The zones where numerical divergence of lift and drag inviscid adjoints is observed, close to the airfoil, are also recalled in the case of a lifting airfoil (avoiding marginal cases like symmetric airfoil and flow):

– for a subsonic flow, Λ_{CD_p} does not exhibit numerical divergence whereas Λ_{CL_p} does at the stagnation streamline and at the wall;

– for a transonic flow for which a shock wave foot is located upstream the trailing edge, Λ_{CD_p} and Λ_{CL_p} exhibit numerical divergence at the stagnation streamline and at the wall;

– for a transonic flow for which all shock wave feet are located at the trailing edge, Λ_{CD_p} and Λ_{CL_p} do not exhibit numerical divergence;

- for a supersonic flow with a detached shock wave and shocks based on the trailing edge, Λ_{CD_p} and Λ_{CL_p} do not exhibit numerical divergence.

5.2. Supersonic regime

We first consider a supersonic flow around the NACA0012 airfoil with a free-stream Mach number $M_{\infty} = 1.5$ and an angle of attack $\alpha = 1^{\circ}$.

The direct solution is displayed in Fig. 3. The flow is supersonic and constant up to a detached shock wave. Downstream the shock wave, the flow is subsonic in a small bubble close to the airfoil leading edge and supersonic elsewhere. It accelerates along the airfoil up to a fishtail shock wave from the trailing edge. Downstream this second shock wave, the flow is still supersonic with a Mach number close to the upwind far field Mach number.

5.2.1. Lift and drag adjoint solutions

Figure A.21 presents the contours of the four components of the adjoint field. The gradient of the discrete adjoint is then evaluated at cell centers using a Green formula and the residual in cell (i, j) of the continuous adjoint equation,

$$res_{ij} = -A_{ij}^T \left(\frac{\partial \Lambda}{\partial x}\right)_{ij} - B_{ij}^T \left(\frac{\partial \Lambda}{\partial y}\right)_{ij},\tag{44}$$

is evaluated for both functions. In the above equation, A_{ij} and B_{ij} are the Jacobians evaluated with cell-center values. For the sake of validation, both terms of the residual and their sum are plotted separately for the lift, on the 2049×2049 mesh in Fig. 5 (left) and then added in Fig. 4 (top left). The cancellation of almost opposite terms is obvious. The percentage of cells with *|res|* below a threshold is increasing as the mesh is refined.

Nevertheless significant (and increasing) |res| values are observed in Fig. 4 on the finest mesh at the trailing edge and along the Mach lines passing through the trailing edge. In the vicinity of the trailing edge, the exact adjoint is zero downstream the backward characteristics emanating from the trailing edge because no perturbation downstream those lines can affect the pressure on the airfoil profile and, thus, the lift and drag. Upstream those lines, perturbations do

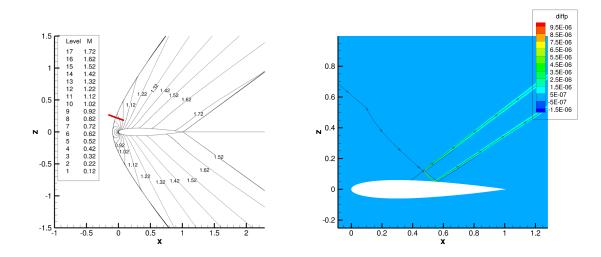


Figure 3: $(M_{\infty} = 1.50, \alpha = 1^{o}, 2049 \times 2049 \text{ mesh})$ Left: contours of Mach number. Right: Change in pressure due to δR^{1} source term ($\epsilon = 6.10^{-6}$) at point (x = 0.4702, y = 0.1184).

affect lift and drag, and thus the adjoints take non-zero values. The corresponding simple discontinuity is more and more accurately captured by any consistent discrete adjoint but the discrete res_{ij} , that is independent of the numerical scheme *R*, exhibits high values along the characteristics passing through the trailing edge.

The dual consistency improvement is also checked quantitatively calculating the mean norm of the *res* components inside a fixed region close to the profile (interior of the $((x-0.5)/0.55)^2 + (z/0.1)^2 = 1$ ellipse and 0.1c upwind the two discontinuous lines issued from the trailing edge or their contribution appears to be overwhelming). These means are then summed using ponderations by the far field velocity to account for the dimension of the components and the resulting all-components residual, denoted *RES*, appears to be decreased by a few percent by the modification of the $F_{3/2}^{JST_c}$ differential for adjoint consistency. More precisely the decrease of *RES* goes form 1.5% (coarsest mesh) to 3.3% (finest mesh) for the lift whereas it goes from 1.4% (coarsest mesh) to 3.8% (finest mesh) for the drag. Concerning far field boundary conditions, the normal Mach number appears to be supersonic at the intersection of the characteristic geometrical strips (see Fig. 5) and the far field boundary. No continuous adjoint boundary conditions is hence to be applied there and no check of discrete versus continuous adjoint is required. Equation (43) is the discrete counterpart of the continuous boundary condition at the wall in (6) and its two terms are plotted in the right part of Fig. 4. They appear to be superimposed, so (43) is actually well satisfied.

5.2.2. Adjoint fields upstream of the shock

The flow is supersonic and constant upstream the detached shock wave. The Jacobians A and B in the continuous adjoint equation (4) are hence constant matrices in this part of the fluid domain and specific analysis of the continuous adjoint solution is possible in this region. These calculations, partly presented in [45], are here further developed and assessed. In a supersonic regime, the direct and adjoint equations both exhibit specific directions of propagation corresponding to simple waves solutions to (4):

$$\psi(x,y) = \phi(x\sin(\zeta) - y\cos(\zeta))\lambda_0,$$

where ζ is the angle made by the direction of propagation with the x-axis, λ_0 is a vector representing the convected information and ϕ is a scalar function. Injecting this expression into (4) yields

$$\phi'(x\sin(\zeta) - y\cos(\zeta)) \times (\sin(\zeta)A^T - \cos(\zeta)B^T)\lambda_0 = 0$$

This equation admits a non-trivial solution λ_0 if and only if det $(\sin(\zeta)A^T - \cos(\zeta)B^T) = 0$ and simple algebraic

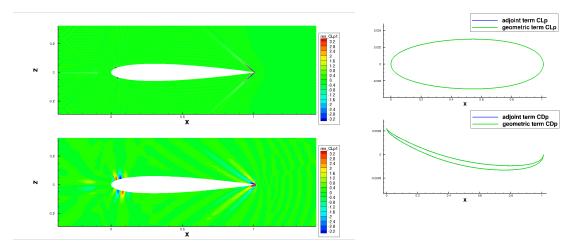


Figure 4: $(M_{\infty} = 1.5, \alpha = 1^{\circ})$ Left: Residual of the continuous equation (first component) evaluated with the lift discrete adjoint fields (bottom: 129×129 mesh, top: 2049×2049 mesh), right: geometric and adjoint terms of equation (43) for lift and drag (2049×2049 mesh)

arguments [45] allow to prove that

$$\begin{aligned} \zeta &= \alpha \quad \text{or} \quad \alpha + \pi \\ \zeta &= \alpha - \mu \quad \text{or} \quad \zeta = \alpha - \mu + \pi \\ \zeta &= \alpha + \mu \quad \text{or} \quad \zeta = \alpha + \mu + \pi, \end{aligned}$$

where α denotes the angle of attack (so $u_x = \|\overline{U}\|\cos(\alpha)$ and $u_y = \|\overline{U}\|\sin(\alpha)$) and $\mu = \arcsin(1/M_{\infty})$ is the Mach angle. Hence, the information propagates along the three privileged directions $\zeta = \alpha$, $\zeta = \alpha - \mu$ et $\zeta = \alpha + \mu$. Evidently, the domains of influence and dependency are inverse one to another for the state and adjoint variables.

The λ_0 eigenvectors of interest are those of $\sin(\zeta)A^T - \cos(\zeta)B^T$. These are also the left eigenvectors that appear in the more classical diagonalization of the inviscid flux Jacobian. Following [52], the (left) eigenvectors associated with $\zeta = \alpha \pm \mu$ (null eigenvalues $u_x \sin(\zeta) - u_y \cos(\zeta) \mp c$) read

$$\lambda_0^{\alpha-\mu} = \begin{pmatrix} \frac{c}{\rho} \left(\frac{-u_x n_x - u_y n_y}{c} + \frac{(\gamma-1)}{2} M^2 \right) \\ \frac{1}{\rho} \left(n_x - (\gamma-1) \frac{u_x}{c} \right) \\ \frac{1}{\rho} \left(n_y - (\gamma-1) \frac{u_y}{c} \right) \\ \frac{\gamma-1}{\rho c} \end{pmatrix}, \quad \lambda_0^{\alpha+\mu} = \begin{pmatrix} \frac{c}{\rho} \left(\frac{u_x n_x + u_y n_y}{c} + \frac{(\gamma-1)}{2} M^2 \right) \\ -\frac{1}{\rho} \left(n_x + (\gamma-1) \frac{u_x}{c} \right) \\ -\frac{1}{\rho} \left(n_y + (\gamma-1) \frac{u_y}{c} \right) \\ \frac{\gamma-1}{\rho c} \end{pmatrix},$$

for a general direction $(n_x, n_y)^T$, which may be replaced by $(\sin(\zeta), -\cos(\zeta))^T$ to recover the solution as a function of the simple wave angles. Checking that the simple waves solution satisfy relation (18) uses the nullity of the eigenvalue $(u_x n_x + u_y n_y + c = 0$ for the first vector and $u_x n_x + u_y n_y - c = 0$ for the second eigenvector).

The dimension of the eigenspace associated with $\zeta = \alpha$ is two but the classically exhibited left eigenvectors [52] do not satisfy the Giles and Pierce relation for pressure-based outputs (18). The vectors of this 2-D space that satisfy this relation is the 1D space generated by

$$\lambda_0^{\alpha} = \begin{pmatrix} -1 - \frac{(\gamma - 1)}{2} M^2 \\ \frac{(\gamma - 1)u_x}{c^2} + \frac{2n_y}{n_y u_x - n_x u_y} \\ \frac{(\gamma - 1)u_y}{c^2} - \frac{2n_x}{n_y u_x - n_x u_y} \\ -\frac{\gamma - 1}{c^2}. \end{pmatrix}$$

Figure 5 (right) highlights the directions of propagation in the first component discrete adjoint field. The ratio of the adjoint components inside all three geometrical strips is found equal to the ratio of the corresponding components

of the associated λ_0 vector. The final demonstration of the consistency between the discrete adjoint fields and the theoretical form of the continuous adjoint solution upwind the shock wave, is obtained by performing a line extraction of the three terms in

$$\psi(x,y) = \phi_{\alpha}(x\sin(\alpha) - y\cos(\alpha))\lambda_0^{\alpha} + \sum_{\nu=\pm\mu}\phi_{\alpha+\nu}(x\sin(\alpha+\nu) - y\cos(\alpha+\nu))\lambda_0^{\alpha+\nu},$$
(45)

and propagating these values in the complete zone upwind the detached shock wave. More precisely, the values of these terms are extracted from a fine discrete adjoint field at a distance 2.3*c* from the leading edge (where the three bands are separated). They are then interpolated everywhere upwind the shock wave according to the local values of $x\sin(\zeta) - y\cos(\zeta)$, with $\zeta \in \{\alpha, \alpha \pm \mu\}$. For the finer meshes, the resulting field appears to be identical to the actual discrete adjoint field, upstream of the shock wave, where the bands are superimposed (results not shown here).

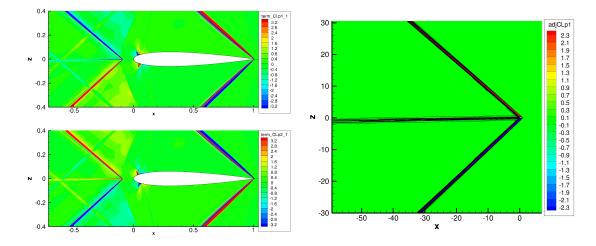


Figure 5: $(M_{\infty} = 1.5, \alpha = 1^{o})$ Top left: $-A^{T}(\partial \Lambda_{CL_{p}}/\partial x)$ discretized with discrete adjoint field (first component). Bottom left: $-B^{T}(\partial \Lambda_{CL_{p}}/\partial y)$ discretized with discrete adjoint field (idem) (2049 × 2049 mesh), right: Far field view of first component of CL_{p} adjoint (4097 × 4097 mesh).

5.2.3. Residual perturbation analysis

When the residual perturbation is located in a supersonic zone, its influence on the flow close to the source appears to be restricted to the downstream part of the streamline and of the two characteristic curves passing by the location of the source. Moreover, assuming a constant flow W, by the same arguments as in previous section, its perturbation δW can be expressed as

$$\delta W(x,y) = \Phi_{\alpha}(x\sin(\alpha) - y\cos(\alpha))r^{\alpha} + \sum_{\nu=\pm\mu} \Phi_{\alpha+\nu}(x\sin(\alpha+\nu) - y\cos(\alpha+\nu))r^{\alpha+\nu}, \tag{46}$$

where ψ_{ζ} , with $\zeta \in \{\alpha, \alpha \pm \mu\}$, stands for a small scalar perturbation and each r^{ζ} vector is a right eigenvector of the Jacobian $\sin(\zeta)A - \cos(\zeta)B$. The consistency of the actual numerical δW with this analytical model can be simply assessed, upwind the detached shock, for δR^1 and δR^2 in (15), since they activate the Mach-lines part of the solution,

$$\Phi_{\alpha-\mu}(x\sin(\alpha-\mu)-y\cos(\alpha-\mu))r^{\alpha-\mu}+\Phi_{\alpha+\mu}(x\sin(\alpha+\mu)-y\cos(\alpha+\mu))r^{\alpha+\mu},$$

with one-dimensional vector spaces span{ $r^{\alpha-\mu}$ } and span{ $r^{\alpha-\mu}$ }: it was successfully verified that the ratio of the components of the discrete δW^1 and δW^2 is the one of the corresponding right eigenvector (results not shown here).

On the contrary, if a δR^1 , δR^2 or δR^4 source term is located in the subsonic bubble or if one of the three curves enters the subsonic bubble, then the support of the flow perturbation includes this complete subsonic area in agreement

with the elliptic nature of the equations [63, chap. 11]. A δR^3 perturbation, conversely, affects the region along the streamline downstream the location of the source, even if located in a subsonic zone.

More details are now given for the case where the source term is located in the supersonic zone. Let consider the decomposition (46) of the perturbation. If the entropy or the total enthalpy (that are convected in steady state Euler flows) are perturbed (δR^3 or δR^4), close to the source, the perturbation is located along the trajectory downstream the source and possibly along shock waves for δR^4 . If these quantities are not altered by the perturbation (δR^1 or δR^2), the response of the steady state flow to the perturbation, close to the source, is located along the two characteristic lines downstream the source and the usual relative-variations along trajectories of thermodynamic and kinetic variables are valid between nominal and locally perturbed flow. More precisely ²:

- δR^1 induces no change in the stagnation quantities and entropy. The Mach number decreases along the two characteristic lines starting from the location of the perturbation. The static pressure, temperature and density increase and velocity components are also perturbed along these two lines with a reduction of the velocity magnitude;
- δR^2 induces no change in the stagnation quantities and entropy. Along the upper characteristic curve starting from the perturbation point, the static pressure, density, temperature increase, whereas the Mach number, velocity magnitude, and x-component of velocity decrease. Opposite variations are observed along the lower characteristic curve. The y-component of the velocity increases along both characteristic curves;
- δR^3 induces no variation of stagnation pressure, static pressure and Mach number. An increase of total enthalpy (stagnation temperature), temperature, both components of velocity and entropy is observed along the trajectory starting from the location of the perturbation. The density is reduced;
- δR^4 induces no local variation of the static pressure except along shock waves and no variation of the total enthalpy. The Mach number, density, stagnation pressure, stagnation density, and both velocity components increase along the trajectory starting from the location of the perturbation. Entropy and temperature decrease along the trajectory. As mentioned end of § 3.3 this notion of perturbation downstream the source and along a streamtube of the initial flow is only a description at first approximation as the streamtubes structure of a non-constant flow is perturbed by the δR^4 source.

These zones of influence and dependency of the lift and the drag explain in particular the aspect of the discrete adjoint fields close to the trailing edge, that are bounded by the two characteristics curves passing through the trailing edge as seen in Fig. 6. They are also illustrated in Fig. 3(right) presenting the δW^1 perturbation on the pressure field plotted together with the characteristic curves passing by the location of the source.

5.2.4. Adjoint fields across the shock

The adjoint variables are continuous across shocks, whereas their derivatives may be discontinuous [40, 1, 42]. In Fig. 6, a clear discontinuity of the adjoint-drag or the adjoint-lift gradient is observed for the adjoint component associated with *z*-coordinate momentum equation.

Figure 7 validates the jump relations on the adjoint derivatives (10) to (12b) derived in § 2.2 at the discrete level for both lift and drag adjoints. We display here the evolution of the arguments between the jump operator $[\cdot]$ in the jump relations along a line perpendicular to the shock (the line is indicated in red in Fig. 3) which should be continuous across the shock. The normal and tangential derivatives in (10) to (12b) are here given in a frame attached to the shock and evaluated from the discrete adjoint field Λ . The shock location is about s = 0.11 and we observe that the jump relations are well satisfied, while the gradients normal to the shock of the adjoint variables, $\partial_n \Lambda$, display large discontinuities at the shock position.

5.3. Transonic regime

We now consider a transonic flow around the NACA0012 airfoil with conditions $M_{\infty} = 0.85$ and $\alpha = 2^{\circ}$. A strong shock wave develops on the suction side and a weaker shock on the pressure side (see Fig. 8 left).

²all variations are given for a positive ε in equation (15) and positive components of velocity for the nominal flow

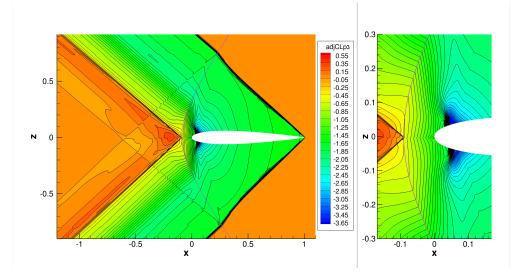


Figure 6: $(M_{\infty} = 1.5, \alpha = 1^{\circ}, 4097 \times 4097 \text{ mesh})$ Contours of the adjoint component associated with *z*-coordinate momentum equation. The position of the shock is indicated by a pink line.

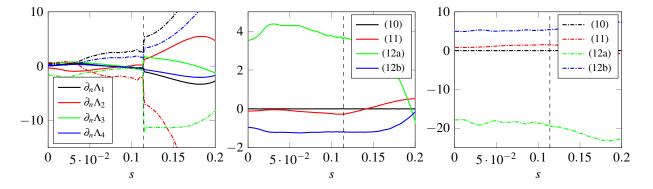


Figure 7: $(M_{\infty} = 1.5, \alpha = 1^{\circ}, 4097 \times 4097 \text{ mesh})$ Evolutions of drag (continuous lines) and lift (dash-dotted lines) adjoint quantities along a straight line across and normal to the upstream shock between points (-0.151, 0.266) and (0.077, 0.184) as a function of the local coordinate *s* (the line is indicated in red in the Mach number contours of Fig. 3). An equation number refers to the arguments between brackets $[\cdot]$ in the corresponding equation, that should be continuous across the shock, e.g., $v_n(\partial_n \Lambda_1 - H \partial_n \Lambda_4)$ has been plotted for (10).

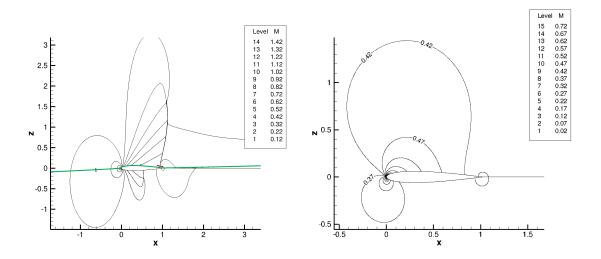


Figure 8: (4097×4097 mesh) Contours of Mach number. Left: $M_{\infty} = 0.85$, $\alpha = 2^{\circ}$, right: $M_{\infty} = 0.4$, $\alpha = 5^{\circ}$.

5.3.1. Lift and drag adjoint solutions

Figure A.22 presents the contours of all four components of the drag and lift adjoint fields. As indicated before, the choice of the scale for the contours of first and last adjoint components in Figs. A.21, A.22 and A.23 allows to visually check that (18) is well satisfied by the discrete adjoint fields. Both fields exhibit strong values and gradients close to the wall, the stagnation streamline, the two characteristics impinging the upper side and lower shock foot and two other characteristic curves that form a circumflex with the previous two. These features have been observed previously [8, 45, 43, 42].

The physical point of view of Giles and Pierce [1] recalled in § 3.3 is used again and the δCL_p^d terms corresponding to the four source terms in (15) are plotted in Fig. A.15. In the sense of equations (16)-(17) the strong values and gradients of δR^1 and δR^2 along the characteristic curves that form the two circumflex correspond to those of Λ_{CLp} . Accordingly, the high values and gradients of δR^4 located close to the wall or to the stagnation streamline correspond to those of Λ_{CLp} . The asset of this approach is obvious when studying the singular behavior of the adjoint fields: the $\delta J^{1 \le d \le 4}$ responses to the physical source terms exhibit only part of the singular zones of the classical adjoint fields and the high values/gradients of one δJ^d are transferred to all or to several of the usual adjoint components according to equation (17).

The residuals of the continuous adjoint equation are evaluated by using the method introduced in § 5.2.1. As the mesh is refined, the zones with significant residuals have a decreasing area but remain visible. Increasing values are also observed close to the wall, the stagnation streamline and the characteristic line that impacts the upper side shock foot, that are known to be zones of large values and large gradients for the lift and drag adjoints [45, 43, 42] as highlighted in the left part of Fig. 9. The far field adjoint boundary condition is satisfied by the discrete adjoint fields as the adjoint field is almost zero at the far field boundary. Right part of Fig. 9 illustrates the verification of continuous-like adjoint wall boundary condition. It is observed that (43) is satisfied except at the shock feet and the trailing edge. At the shocks feet, the first differences in neighboring Λ along the wall in (39) and (40) may be too large for a simple lower-order spatial analysis. At the trailing edge, the divergence of the discrete adjoint momentum components and the discontinuity of Λ_{CDp_2} and Λ_{CLp_2} between upper side and lower side (see Fig. A.23) may explain the observed behavior.

5.3.2. Numerical assessment of exact discrete adjoint and modified consistent adjoint

The transonic test case is retained for the assessment of the exact discrete adjoint in our code [59, 62]. Also tested is the accuracy of the gradients when the Jacobian modification for consistency is applied.

First, a series of ten symmetric bumps with 0.4*c* span is considered. The wall mesh is deformed normally according to $\exp(-0.25(s_{bmax} - s_{bmin})^2/((s - s_{bmin})(s_{bmax} - s)))$. In the fluid domain, the mesh deformation follows the

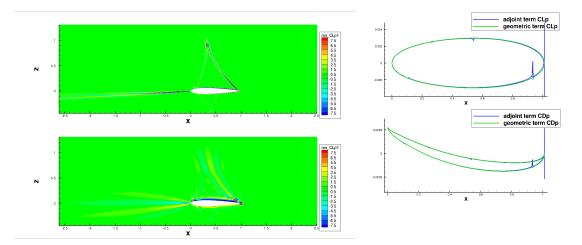


Figure 9: $(M_{\infty} = 0.85, \alpha = 2^{\circ})$ Left: residual of the continuous equation (first component) evaluated with the lift discrete adjoint fields (bottom: 129×129 mesh, top: 2049×2049 mesh). Right: geometric and adjoint terms of (43) for lift and drag (2049×2049 mesh).

normal vector at the closest point of the wall and the displacement amplitude is smoothed from maximum value at the wall, to zero at the distance 0.4c. The ten bumps are applied with small positive and negative increments to the (513×513) mesh and steady state simulations are run to produce reference lift and drag derivatives. The lift and drag gradients are calculated besides using the exact discrete adjoint, the modified discrete adjoint for consistency and the discrete adjoint without linearization of the spectral radius and the sensor [58]. All gradient values are gathered in table A.1. Considering lift gradients, the mean error for exact linearization is less than 0.1% (and calibration of the finite-difference step may improve this accuracy) whereas it is 11.5% for the modified dual consistent version. This 11.5% error is close to the 10.6% error obtained with the frozen sensor and frozen spectral radius approximation, and indicates that this gradient may be involved in actual adjoint based shape optimization although probably not with best efficiency. Similar conclusions may be drawn from the drag gradients.

Besides, the agreement between the linear and the non-linear source term approaches is checked. Let us recall that the linear approach just calculates $(\delta J_m^1, \delta J_m^2, \delta J_m^3, \delta J_m^4)$ from the standard adjoint fields using equation (16) whereas the non-linear approach consists of adding one of the source terms $\delta R^l - eq$. (15) – to the scheme flux balance, for a specific cell *m*, running a steady state simulation and calculating δJ_m^l as the difference of the resulting J^l with its nominal evalutation. Note that, as above with the calculation of the shape optimization gradients, any error in the scheme Jacobian $\partial R/\partial W$ would become apparent with this second type of comparisons. The non linear approach is obviously expensive and can only be tested for a limited number of cells. It has been applied for the fourth source term δR^4 , for two series of cells, upper-side close to the wall at $x \simeq 0.5$ and close to the stagnation streamline at $x \simeq -0.6$. The value of ε and the number of iterations have been chosen such that the first four significant numbers of the functions of interest do not change and the next four or five significant numbers are known upon reaching the steady-state, at the end of the perturbed calculation. The comparison between the linear (red curve) and non linear (green squares) values is presented in Fig. A.17. The agreement is very good and allows to use the mechanical perturbations induced by the source terms (15) to discuss properties of $(\delta J_1^n, \delta J_m^2, \delta J_m^3, \delta J_m^4)$ and then move to properties of the standard adjoint fields. This is done hereafter only for $\delta R^4 / \delta J^4$.

5.3.3. Influence of a δR^4 perturbation in the vicinity of the wall and the stagnation streamline

As mentioned in § 5.3.1, considering the physical source terms first – equation $(17) - \delta R^4$ is the only physical source "responsible" for high values of lift/drag-adjoint and gradient of adjoint close to the wall and the stagnation streamline. The mechanism by which δR^4 modifies the flow field and the forces values is discussed here for the vicinity of the stagnation streamline and the wall (upper side) using the non-linear approach which accuracy has just been discussed.

In the first series of considered perturbed flows, the δR^4 source terms are located on the upper side in the supersonic

area, along a mesh line perpendicular to the wall and close to x = 0.5. In a supersonic zone, the perturbation of the flow caused by a δR^4 source term along the corresponding streamline has been described in § 5.2.3: no local variation of the static pressure (except along shock waves - see below) and no variation of the total enthalpy are observed whereas the Mach number, the density, the stagnation pressure, stagnation density and the velocity are increased along the trajectory starting from the location of the perturbation. Hence, for the almost normal upperside shock, the classical equation for the ratio of downwind over upwind static pressure as a function of the upwind Mach number cannot be satisfied where the perturbed streamline hits the shock with an increased Mach number. In fact in the perturbed flow, the upper side shock is moved upstream and the shifted shock goes with a decreasing upwind static pressure and an increasing downwind static pressure. It is observed that the smaller the distance of the source and perturbed streamline to the wall, the larger the displacement of the upper side shock foot which explains the growth of δCL_{P_4} in the vicinity of the wall. Observing the static pressure changes at smaller scales, it is noted, as expected, that the perturbation of the static pressure in the subsonic area is not restricted to the continuation of the streamline but extends to the whole subsonic area close to the profile downstream the shocks. Regarding the static pressure close to the lower side, at these finer scales, an increase is observed upwind the shock and below the trailing edge whereas a decrease is observed downwind the shock; this goes with a backward displacement of the lower shock. Both changes of the static pressure at the wall correspond to an increase of the lift that is consistent with the local values of δCLp^4 . To complement this description, the fraction of the forces variation due to the two shocks displacement is calculated for all source points of the series (Fig. A.17 left). The pressure difference w.r.t. the nominal pressure is summed along 36 faces only among the 2048 of the wall mesh in the vicinity of the shock waves ($x \in [0.535,0555]$ lower side and $x \in$ [0.925,0945] upperside) and is then divided by the total change in the function estimate. For the lift, theses ratios are included in [0.806, 0.921] with a mean value of 0.880. For the drag, the corresponding interval is [0.925,1.038] and the mean value is 0.985. This confirms the main effect of the displacement of the two shocks.

If the δR^4 source is located close to the wall but downwind the upper side shock, similar shock displacements and lower side fine scale perturbations of the pressure are observed. On the contrary, the flow perturbations created downwind the upper side shock are very different for sources located on the same streamline either sides of the shock.

Concerning the points located close to the stagnation streamline, the mechanism that produces the lift perturbation δCLp^4 due to the δR^4 source also seems to be correlated with convection since the iso- δCLp^4 roughly follow the streamlines (see Fig. A.15 right). Of course, the increment of stagnation pressure and stagnation density, and the decrease of entropy are convected from the location of the source where they have been created (see Fig. 10). Surprisingly, although the source is now located in a subsonic zone, the main change in the velocity and Mach number fields also occur along the trajectory. These increments being propagated up to the upper side shock, the mechanism through which both shocks are moved is then the one described before. This description is complemented with the ratios of the function variations that result from the changes in the pressure in the vicinity of the shocks only ($x \in [0.535,0555]$ lower side and $x \in [0.925,0945]$ upperside) divided by the corresponding total variation. The considered points are those appearing in the right part of Fig. A.17 ($x \simeq -0.6 \ y \simeq -0.04$) at a distance lower than 0.025*c* to the stagnation streamline. For the lift, theses ratios are included in [0.793, 1.245] with a mean value of 0.882. For the drag the interval is [0.762,0.907] and the mean value is 0.840. Again, the dominant influence of shock displacement in the lift and drag variation is confirmed.

Finally, we would like to investigate whether the influence of δR^4 is evolving smoothly from the vicinity of the stagnation streamline to the vicinity of the wall. We have already mentioned the pros (the main process is the convection of the source perturbation) and cons (the streamline structure of the original flow is not strictly preserved) of a positive answer to this question. It is investigated numerically extracting δCLp^4 and δCDp^4 along a streamline close to the stagnation streamline and the upperside wall (see Fig. 8 then Fig. A.18 – the gaps between the curve and the non-linear verification calculations come from the fact that not all the selected cells are exactly crossed at their center by the streamline). The δCLp^4 curve of Fig. A.18 is completed in Fig. A.19 with its counterparts on a finer and a coarser mesh and it is checked that the general shape of these curves is not affected by the mesh size. The levels of δCLp^4 seen in Fig. A.18 upwind the airfoil at x \simeq -0.1 are observed along the wall but a downwards oscillation just upwind the profile makes it difficult to give a sure conclusion.

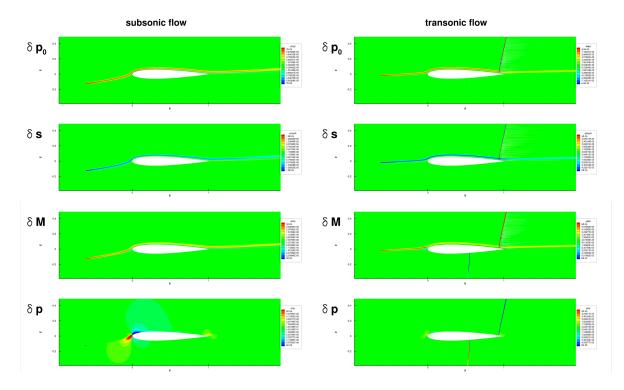


Figure 10: (2049×2049 mesh) Difference in stagnation pressure, entropy (divided by the adiabatic exponent), Mach number and static pressure w.r.t. nominal flow due to δR^4 . Left: $M_{\infty} = 0.4$, $\alpha = 5^o$, source at point (-0.612,-0.127). Right: $M_{\infty} = 0.85$, $\alpha = 2^o$, source in (-0.623,-0.020).

5.3.4. Asymptotic behavior of lift and drag adjoint at the stagnation streamline and the wall

In [1], the authors consider a 2-D inviscid flow about an airfoil and an output J defined as the integral along the wall of the pressure times a local factor. With the additional approximation of potential flow, they derive the asymptotic behavior of δJ_m^4 , the variation of J due to δR^4 , when the source term is located in the vicinity of the stagnation streamline: under this potential flow assumption, they prove that $\delta J^4 \simeq \pm d^{-1/2}$ where d is the distance of the source m to the stagnation streamline and the sign is changed when crossing the streamline. This relation is not always numerically well satisfied by numerical lift / drag adjoint fields of compressible Euler flows [43, 42].

For the transonic test-case of interest, δCLp_m^4 and δCDp_m^4 seem to result of similar convective perturbations of the flow for points m located close to the stagnation streamline and close to the wall upwind the shock. Using the structured and regular meshes from [60], one may evaluate the φ exponent such that $\delta J^{\bar{4}} \simeq d^{\varphi}$ in the vicinity of the wall. This exponent appears to depend on the x location (rather than on CD vs CL, lower side vs upper side). It is decreasing with increasing x, from 0. at the leading edge to about -0.1 at x = 0.8 and then more rapidly when moving closer to the trailing edge. (Curves not shown here because changing the mesh density, the $F_{3/2}^{JST}$ formula or selecting its adjoint-consistent linearization instead of its exact linearization, significantly modifies these curves although not the decreasing trend from a null value.)

Finally the values of δCLp^4 are extracted along the wall on the finest used meshes (Fig. A.20). They appear to grow as the cells adjacent to the wall get thiner coherently with the similar behavior observed for the lift or drag adjoint components in other publications ([42] fig. 12, [64] fig. 1.1). As the wall boundary condition that involes a linear boundary combination of Λ_2 and Λ_3 , is numerically well satisfied (equation (43) and fig. 9 right), this is surprising although not impossible: it should be noted that in the vicinity of a wall, with local normal vector (n_x, n_y) , it is worthwhile to calculate the linear combination of the second and third columns of equation (17) by (n_x, n_y) to show that the term involving δCLp_4 in $\Lambda_2 n_x + \Lambda_3 n_y$ is $-\gamma p_0/c^2(u_x n_x + u_y n_y)\delta CLp_4$ with $(u_x n_x + u_y n_y) \rightarrow 0$. We have checked also that this behavior close to the wall is not an artefact due to numerical dissipation by performing calculations with different k^4 . The influence of the cell-height at the wall always dominates the one of the artificial dissipation and, for a given mesh density, the largest values of δCLp^4 are obtained for the lowest k^4 .

5.3.5. Adjoint fields across the shock

Figure 11 highlights a clear discontinuity across the shock of the gradient of the drag or the lift adjoint component associated with the z-coordinate momentum. This is further analyzed in Fig. 12 where the arguments in the brackets in (10) to (12b) are plotted along the line displayed in Fig. 8 (left) that crosses the shock. Again, it is observed that the jump relations (10) to (12b) are well satisfied while the adjoint derivatives in the direction normal to the shock, $\partial_n \Lambda$, are discontinuous across the shock.

5.4. Subsonic regime

Finally, we consider a smooth subsonic flow with free-stream conditions $M_{\infty} = 0.4$ and $\alpha = 5^{\circ}$. The Mach number contours are presented in Fig. 8 where we observe the stagnation point located in the lower part of the leading edge as well as a strong acceleration of the flow on the upper side due to the profile incidence.

5.4.1. Lift and drag adjoint solutions

Figure A.23 presents the contours of all four components of the adjoint fields. The lift adjoint components exhibit strong values and gradients close to the wall and the stagnation streamline. The amplitudes of these values increase as the mesh is refined. Conversely, all components of the drag adjoint appear to be bounded and to converge as the mesh is refined. For this flow without shocks, these different behaviors may be attributed to the facts that the adjoint field quantifies the sensitivity of the quantity of interest w.r.t. the residuals, and that the limit inviscid drag is zero for a subsonic flow whereas the limit lift is not.

The residuals of the continuous adjoint equations have been evaluated as detailed in § 5.2.1. As the mesh is refined, the zones with significant residuals for the lift-adjoint have a decreasing support but exhibit increasing values close to the wall and to the stagnation streamline (see left part of Fig. 13). The far field adjoint boundary condition is satisfied by the discrete adjoint fields as the adjoint field is almost zero at the far field boundary. Right part of Fig. 13 shows that the adjoint wall boundary condition (43) is well satisfied for both lift and drag. The approximate linearization for consistency of $F_{3/2}^{JST_c}$ proposed in §4.5 is assessed quantitatively for *CDp* (*CDp* only

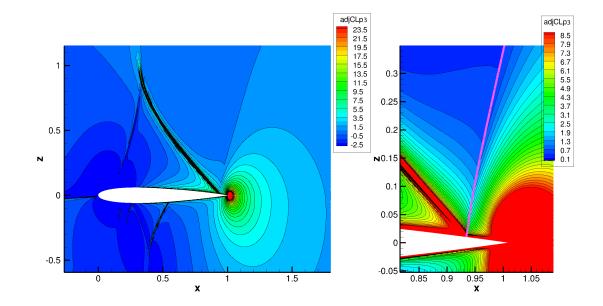


Figure 11: ($M_{\infty} = 0.85$, $\alpha = 2^{\circ}$, 4097 × 4097 mesh) Contours of adjoint component associated with the *z*-coordinate momentum equation (sonic line in pink).

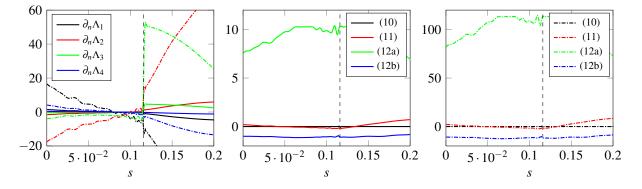


Figure 12: $(M_{\infty} = 0.85, \alpha = 2^{\circ}, 4097 \times 4097 \text{ mesh})$ Evolutions of drag (continuous lines) and lift (dash-dotted lines) adjoint quantities along a straight line across and normal to the upper shock between points (0.865, 0.064) and (1.016, 0.038) as a function of the local coordinate *s* (the line is indicated in red in the Mach number contours of Fig. 8). An equation number refers to the arguments between brackets [[·]] in the corresponding equation, that should be continuous across the shock, e.g., $v_n(\partial_n \Lambda_1 - H \partial_n \Lambda_4)$ has been plotted for (10).

as the adjoint of *CLp* is numerically diverging) calculating the mean norm of the *res* components inside a fixed region close to the profile (interior of $((x - 0.5)/0.55)^2 + (z/0.1)^2 = 1$ ellipse excluding a 0.005c circle about the trailing edge or the contribution of the trailing edge vicinity appears to be dominant). These means are then summed in the aggregate residual denoted *RES*. As in the supersonic case, it appears to decrease be a few percent by the modification of the $F_{3/2}^{JST_c}$ differential for adjoint consistency. More precisely, *RES* is decreased by 2.6% (coarsest mesh) to 5.0% (finest mesh).

The physical point of view of Giles and Pierce [1] is then considered to gain understanding in the behavior of the lift-adjoint. The δCLp^1 , δCLp^2 , δCLp^3 , and δCLp^4 responses have been calculated and plotted in Fig. A.16. We observe that δR^4 is the only source responsible for the singular behavior of the adjoint-lift close to the wall and stagnation streamline.

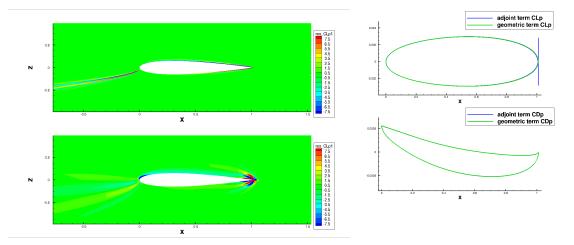


Figure 13: ($M_{\infty} = 0.4, \alpha = 5^{\circ}$) Left: residual of the continuous equation (first component) evaluated with the lift discrete adjoint fields (bottom: 129×129 mesh, top: 2049×2049 mesh). Right: geometric and adjoint terms of equation (43) for lift and drag (2049×2049 mesh).

5.4.2. Influence of a δR^4 perturbation in the vicinity of the wall and the stagnation streamline

As in transonic and supersonic flows, a δR^4 source results in positive increments in the stagnation pressure and stagnation density and a negative increment in entropy. All three increments are convected downstream the location of the source following the classical laws for Euler flows with uniform total enthalpy. However, the response of the subsonic flow to the local perturbation of these three quantities, is very different from the one described in § 5.3.3 for the transonic flow: density, velocity, static pressure and all dependent variables exhibit a global perturbation (see Fig. 10). When the source is located close to the stagnation streamline, the perturbation is maximum close to the leading edge. If it is located just under (resp. above) the stagnation streamline, the main effect on the static pressure at the wall is a decrease all along the pressure (resp. suction) side consistently with the local sign of δCLp^4 (Fig. A.16 right and Fig. 14).

As in the transonic case, we examine if $\delta CLp^4 \simeq d^{\varphi}$ in the vicinity of the wall. Once again, a negative φ exponent decreasing from 0 to about -0.40 when increasing x is derived from this assumption (Not shown here because, as in the transonic test case, changing the mesh density, the $F_{3/2}^{JST}$ formula or selecting its adjoint-consistent linearization instead of its exact linearization, significantly modifies this curve although not the decreasing trend from a null value.)

6. Conclusion

In this work, we address open questions in the field of discrete and continuous adjoint equations for the compressible inviscid flows. The results are illustrated through in-depth numerical experiments on lift- and drag-adjoint fields for lifting flows about the NACA0012 airfoil in supersonic, transonic and subsonic regimes.

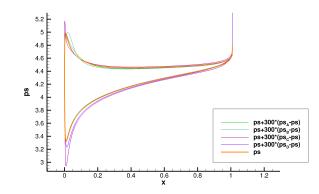


Figure 14: ($M_{\infty} = 0.4$, $\alpha = 5^{\circ}$, 2049×2049 mesh) Pressure at the wall. Influence of δR^4 source term located at points A, B, C, D, on the static pressure at the wall. Distance of points A, B, C, D to the leading edge $\simeq 0.6$. Respective distance to stagnation line is 0.0400, 0.0187 (trajectory to lower side), 0.0181, 0.397 (trajectory to upper side).

We first investigate the dual consistency of the JST scheme in cell-centered FV formulation for the discretization of the compressible 2-D Euler equations. Dual consistency of the scheme is proven at interior cells, while inconsistency may occur at the penultimate cell close to a physical boundary depending on the selected locally modified AD formulas. Two classical and robust AD discretizations at the borders have been proven to be dual-inconsistent and we propose a slight modification of the exact scheme differentiation w.r.t. the penultimate cell flow variables to recover consistency. The implementation of this modification has been carried out in our code and appears to locally improve the regularity of the adjoint field and to speed up their convergence at wall boundaries under grid refinement.

Second, a new heuristic method has been proposed to discuss the adjoint consistency of discrete adjoint fields. It consists of discretizing the continuous equation with the discrete flow and discrete-adjoint field and evaluating the convergence of the residual as the mesh is refined. Coherently with the demonstrated property of adjoint consistency, these residuals have been found to vanish except in areas where: (i) a discontinuous adjoint field is expected (e.g., in the vicinity of the trailing edge for supersonic flows); (ii) the discrete adjoint field exhibits increasing values and gradients where theoretical divergence is suspected (stagnation streamline, wall, specific characteristic lines in supersonic areas).

Third, we derive the general adjoint Rankine-Hugoniot relations across a shock and give relations linking the normal derivatives across the shock. These relations have been numerically validated for a supersonic and a transonic flow.

We then use these tools for the analysis of the lift and drag adjoint fields about the NACA0012 at three flow conditions and, in particular, the analysis of the zones where increasing values and gradients of the adjoint fields are observed when the mesh is refined [1, 43, 42, 65]. The source term approach of Giles and Pierce [1] is recalled and after assessing it for our code w.r.t linear results - Fig. A.17 - it is exploited to analyse the lift and drag adjoint behavior in the vicinity of the stagnation streamline and the wall for the transonic test case. The novelty is for the transonic regime in the detailed description of the flow perturbation resulting of the involved source term : a pertubation along streamline passing by the source results in the displacement of the shocks. The mechanism is similar with a source close to the stagnation streamline or close to the wall so that our numerical results suggest that the behavior of the adjoint fields in the vicinity of the stagnation streamline (where the authors of [1] predicted a numerical divergence under simplifying assumptions) and in the vicinity of the wall are identical. Also explained by this analysis (although not illustrated here) is the well-known difference of numerical behavior in lift or drag adjoint at high transonic Mach numbers (shock-wave feet at trailing edge, no possible shock-foot displacement, no adjoint numerical divergence) and lower transonic Mach numbers (more upwind shock wave feet locations, shock feet displacement under the influence of δR^4 , adjoint numerical divergence). In subsonic regime, the fourth source term proposed in [1] results in a numerically diverging perturbation of the lift, also when approaching the wall or the stagnation streamline, but through a global change of the wall pressure.

Future work will concern the extension of this analysis to laminar flows considering the usual FV cell-centered discretizations of the viscous flux.

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Biblography

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Appendix A. Additional figures and arrays

reference	Bl_1	Bl_2	Bl_3	Bl_4	Bl_5	Bu ₅	Bu_4	Bu ₃	Bu_2	Bu_1
$10^2 (dCLp/da_i)_{f.d.}$	-8.64	-4.86	-5.34	-1.10	-4.78	-1.84	-1.04	-1.32	-2.74	-1.50
$10^2 (dCLp/da_i)_{adj.}$	-8.67	-4.87	-5.36	-1.10	-4.78	-1.84	-1.04	-1.32	-2.74	-1.50
$10^2 (dCLp/da_i)_{c.adj.}$	-7.69	-4.09	-4.80	-1.39	-4.84	-1.85	-1.02	-1.28	-2.58	-0.91
$10^2 (dCLp/da_i)_{adj.fr.}$	-7.68	-4.36	-4.75	-0.87	-4.59	-1.92	-0.98	-1.22	-2.55	-1.86
$10^3 (dCDp/da_i)_{f.d.}$	-6.47	-4.15	-8.32	4.14	9.57	5.45	2.63	0.0892	-1.52	-3.58
$10^3 (dCDp/da_i)_{adj.}$	-6.49	-4.16	-8.33	4.15	9.57	5.45	2.63	0.0867	-1.52	-3.58
$10^3 (dCDp/da_i)_{c.adj.}$	-5.70	-3.53	-7.88	3.91	9.57	5.45	2.65	0.0125	-1.39	-3.10
$10^3 (dCDp/da_i)_{adj.fr.}$	-5.57	-3.69	-7.78	4.33	9.72	5.37	2.67	0.0165	-1.35	-3.90

Table A.1: $(M_{\infty} = 0.85, \alpha = 2^{\circ}, 513 \times 513 \text{ mesh})$ lift and drag gradient w.r.t. parameters driving the amplitudes of ten bumps. Finite-differences (f.d.), exact discrete adjoint (adj.), consistent adjoint (c.adj.), discrete adjoint with frozen κ and ν (adj.fr.)

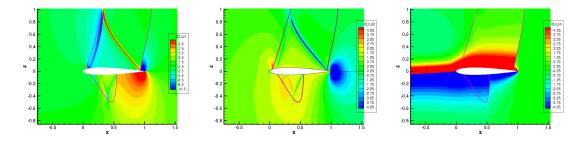


Figure A.15: $(M_{\infty} = 0.85, \alpha = 2^{\circ}, 2049 \times 2049 \text{ mesh})$ Contours of $\delta CL_p^1, \delta CL_p^2, \delta CL_p^4$ (equations (15) and (16) with $\varepsilon = 1$). δCL_p^3 is zero.

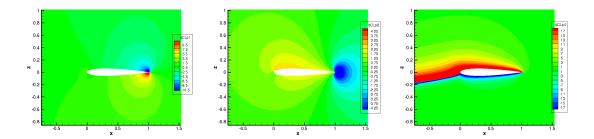


Figure A.16: $(M_{\infty} = 0.4, \alpha = 5^{\circ}, 2049 \times 2049 \text{ mesh})$ Contours of $\delta CL_p^1, \delta CL_p^2, \delta CL_p^3, \delta CL_p^4$ (equations (15) and (16) with $\varepsilon = 1$). δCL_p^3 is zero.

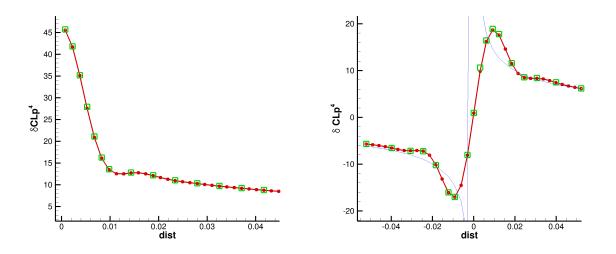


Figure A.17: $(2049 \times 2049 \text{ mesh}) M_{\infty} = 0.85$, $\alpha = 2^{\circ}$. Linear (red curve) and non-linear (green squares) estimations of δCL_p^4 . Left: upper side at the wall $x \simeq 0.5$. Right: in the vicinity of the stagnation streamline $x \simeq -0.6$ (dist being a signed distance to it). The blue curve is a tentative fit with $Ksgn(dist)/\sqrt{|dist|}$ ([1]). The extraction lines are drawn in Fig. 8 left.

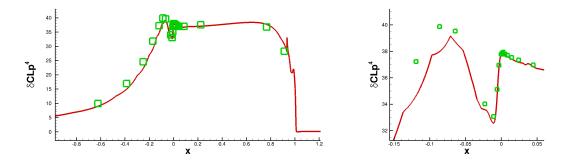


Figure A.18: $(2049 \times 2049 \text{ mesh}) M_{\infty} = 0.85$, $\alpha = 2^{\circ}$. Linear (red curve) and non-linear (green squares) estimations of δCL_p^4 along the streamline passing by (-0.6224,-0.0383). The mean distance of this streamline to the stagnation streamline is about 0.02c. Its distance to the upperside wall is about 0.015c. The shock foot abscissa is $x \simeq 0.935$ (upwards oscillation right of the last green square). The streamline is drawn in Fig. 8 left.

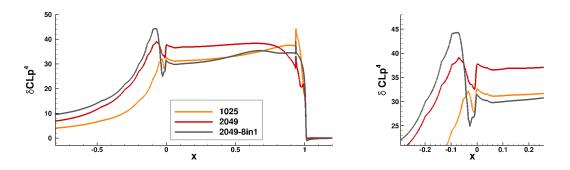


Figure A.19: $M_{\infty} = 0.85$, $\alpha = 2^{\circ}$. Exact discrete adjoint δCL_p^4 along the streamline passing by (-0.6224,-0.0383) for the finest meshes. The mesh denoted 2049-8in1 is a 2049 × 2049 mesh built by regular linear interpolation inside the standard 2049 × 2049 mesh. It is stretched at the wall, the aspect ratio of the cells adjacent to the wall being 1 to 8. (Not shown for the 4097×4097 mesh for which the trajectory is a bit different and higher values are obtained.)

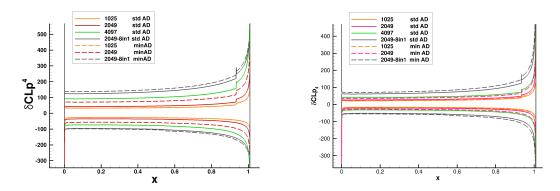


Figure A.20: (finer meshes) $M_{\infty} = 0.85$, $\alpha = 2^{\circ}$. $\delta CLp4$ in the cells adjacent to the wall (equations (15) and (16) with ε =1). Left: exact discrete adjoint. Right: consistent adjoint. The solid line curves correspond to the calculations presented elsewhere ("standard AD" coefficient $k^4 = 0.032$). The dashed line curves correspond to calculations with halved artificial dissipation ("minimum AD" coefficient k4=0.016). This small coefficient does not allow a proper flow convergence with the 4097×4097 mesh.

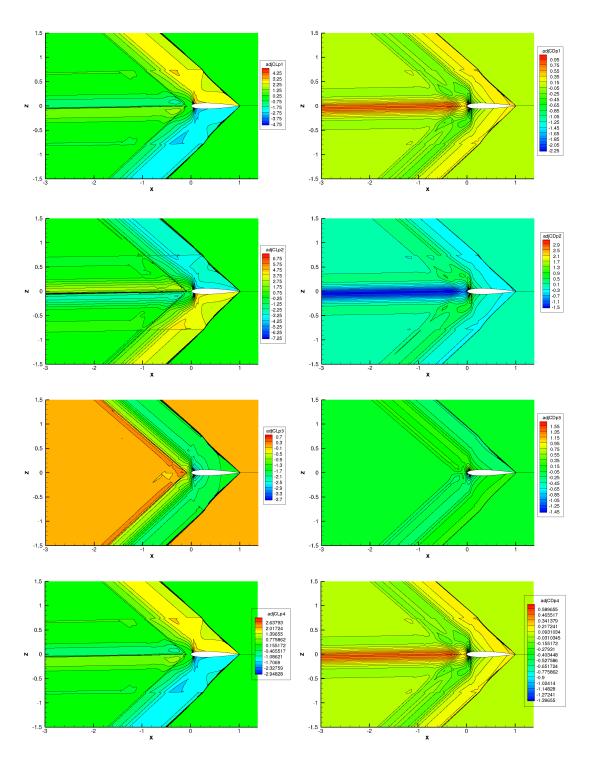


Figure A.21: ($M_{\infty} = 1.5$, $\alpha = 1^{o}$, 4097×4097 mesh) Left: lift adjoint, right: drag adjoint.

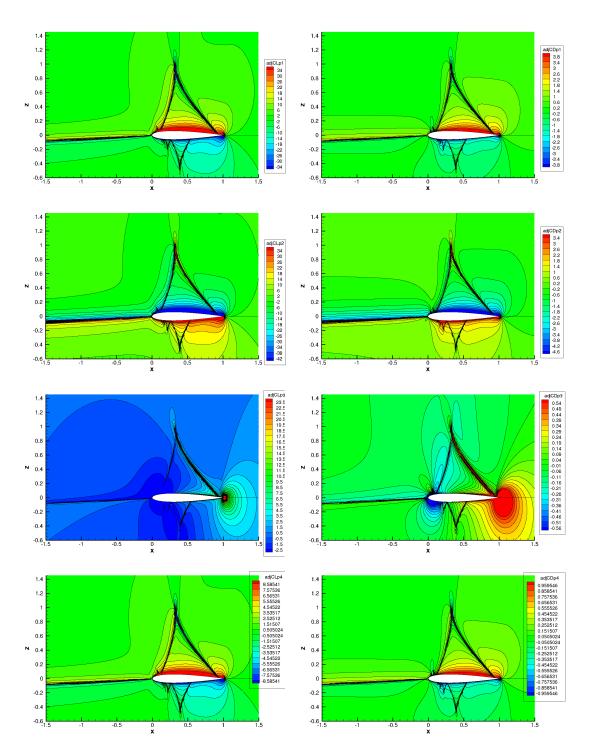


Figure A.22: ($M_{\infty} = 0.85$, $\alpha = 2^{\circ}$, 4097×4097 mesh) Left: lift adjoint, right: drag adjoint.

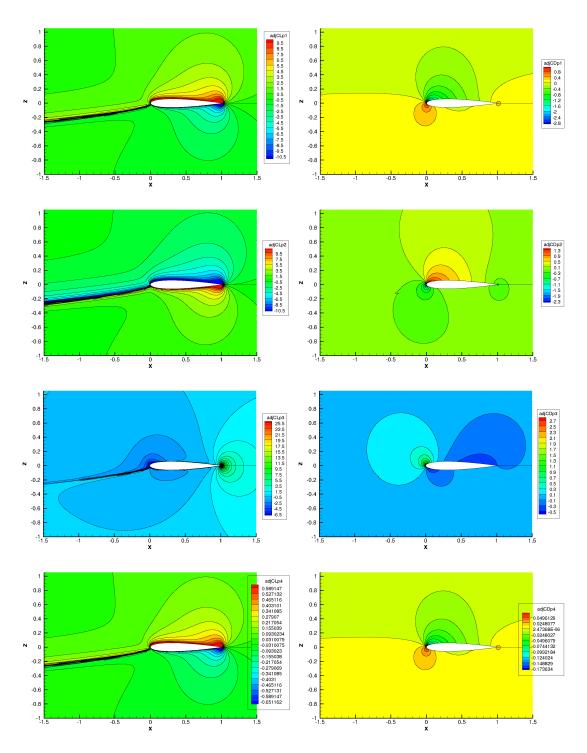


Figure A.23: ($M_{\infty} = 0.4$, $\alpha = 5^{o}$, 4097×4097 mesh) Left: lift adjoint, right: drag adjoint.