Adjoint equations in CFD: duality, boundary conditions and solution behaviour

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Abstract

The first half of this paper derives the adjoint equations for inviscid and viscous compressible flow, with the emphasis being on the correct formulation of the adjoint boundary conditions and restrictions on the permissible choice of operators in the linearised functional. It is also shown that the boundary conditions for the adjoint problem can be simplified through the use of a linearised perturbation to generalised coordinates.

The second half of the paper constructs the Green's functions for the quasi-1D and 2D Euler equations. These are used to show that the adjoint variables have a logarithmic singularity at the sonic line in the quasi-1D case, and a weak inverse square-root singularity at the upstream stagnation streamline in the 2D case, but are continuous at shocks in both cases.

1 Introduction

The last few years have seen considerable progress in the use of adjoint equations in CFD for optimal design [1-9]. In all of the methods, the heart of the algorithm is an optimisation procedure which uses an adjoint method to compute the linear sensitivity of an objective function with respect to a number of design variables.

The simplest approach, at least conceptually, to constructing the discrete adjoint equations begins with the nonlinear discrete residual equations arising from a finite volume discretisation of the original fluid dynamic equations,

$$R_h(U_h, \alpha) = 0.$$

Here U_h is the discrete flow solution and α is initially a single design variable. Differentiating with respect to α gives

$$\frac{\partial R_h}{\partial U_h} \frac{dU_h}{d\alpha} + \frac{\partial R_h}{\partial \alpha} = 0,$$

which determines the change in U_h due to a change in α . Given some nonlinear objective function, $I_h(U_h, \alpha)$, which, for example, may be a discrete approximation to the lift or drag on an airfoil, the derivative with respect to α is simply

$$\frac{dI_h}{d\alpha} = \frac{\partial I_h}{\partial U_h} \frac{dU_h}{d\alpha} + \frac{\partial I_h}{\partial \alpha} \\
= -\frac{\partial I_h}{\partial U_h} \left(\frac{\partial R_h}{\partial U_h}\right)^{-1} \frac{\partial R_h}{\partial \alpha} + \frac{\partial I_h}{\partial \alpha} \\
= V_h^T \frac{\partial R_h}{\partial \alpha} + \frac{\partial I_h}{\partial \alpha},$$

where V_h is the solution of the adjoint equation

$$\left(\frac{\partial R_h}{\partial U_h}\right)^T V_h + \left(\frac{\partial I_h}{\partial U_h}\right)^T = 0.$$

The key point is that derivatives of I_h with respect to other design variables can be expressed in a similar manner, using the same adjoint flow solution. The only additional computation for each additional design variable is the evaluation of $\frac{\partial R_h}{\partial \alpha}$ and its vector dot product with V_h . Each of these two steps involves minimal computational effort, and so the overall computational cost is almost independent of the number of design variables.

The adjoint solution also plays a critical role in numerical error analysis, analysing the error in the computed airfoil lift and drag due to the truncation error inherent in the discretisation. The solution error e_h is defined by

$$U_h = U(x_h) + e_h,$$

where $U(x_h)$ is the analytic flow solution evaluated at the discrete grid points. Linearising the residual equations gives

$$R_h(U(x_h)) + \frac{\partial R_h}{\partial U_h} e_h \approx 0,$$

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where $R_h(U(x_h))$ is the vector of truncation errors obtained by substituting the analytic solution into the discrete residual operator.

If I(U) is the scalar quantity of interest (e.g. lift or drag) based on the analytic solution, then the error in the corresponding discrete approximation, $I_h(U_h)$, can be broken into two components,

$$I_h(U_h) - I(U) = (I_h(U_h) - I_h(U(x_h))) + (I_h(U(x_h)) - I(U)).$$

The second term is the truncation error in approximating the operator I. The first term is due to the error e_h in the discrete solution U_h and can be approximated as follows,

$$I_{h}(U_{h}) - I_{h}(U(x_{h})) \approx \frac{\partial I_{h}}{\partial U_{h}} e_{h}$$

= $-\frac{\partial I_{h}}{\partial U_{h}} \left(\frac{\partial R_{h}}{\partial U_{h}}\right)^{-1} R_{h}(U(x_{h}))$
= $V_{h}^{T} R_{h}(U(x_{h})),$

where the vector V_h is again the adjoint flow solution. Thus the adjoint flow solution relates the errors in quantities such as lift and drag, to the underlying truncation errors in the evaluation of finite volume cell residuals. As well as offering useful bounds on the accuracy of lift and drag predictions, this could also be used as the basis for optimal grid adaptation, giving the most accurate predictions for a given level of computational cost.

This use of the adjoint solution for error analysis has been developed only recently in the CFD community for incompressible flow [10, 11] but there is a longer history of its use for structural analysis [12, 13]. However, in structural analysis one is primarily concerned with point quantities such as peak stresses and so adjoint equation methods are not used widely. In CFD applications, on the other hand, the most important quantities from an engineering perspective are usually integrals and so error analysis and optimal grid adaptation using the adjoint solution offer much more potential.

The above introduction to adjoint equation methods has followed the discrete approach in which one begins with the nonlinear discrete equations and then considers linear perturbations. A drawback of this approach to formulating the adjoint equations is that it does not offer clear insight into the nature of the discrete adjoint solution. The alternative approach is to construct the adjoint p.d.e. together with appropriate boundary conditions, and then discretise that to obtain a discrete adjoint solution. The important advantage of this analytic approach is that the behavior of the adjoint solution can be investigated by considering the adjoint p.d.e. Knowledge of the behaviour of the adjoint solution at a shock or sonic line in compressible flow calculations, or within the boundary layer and wake in viscous flow applications, could be very important in constructing accurate error estimates and for optimal grid refinement and adaptation.

The objective of this paper is to follow this analytic approach to advance the mathematical theory of adjoint equations for CFD applications. The first half of the paper is concerned with the construction of the adjoint formulation. This is achieved within a framework of duality in which the original (primal) and adjoint (dual) formulations are equivalent representations of the same linear problem. The general theory is developed first for a large class of boundary value p.d.e.'s. The theory is then applied to the convection/diffusion, Euler and Navier-Stokes equations in two dimensions.

The second half investigates the behaviour of solutions of the adjoint Euler equations. By expressing the adjoint solution in terms of the Green's function for the original linearised Euler equations, it is shown that the adjoint solution for the quasi-1D Euler equations has a $\log x$ singularity at a sonic line, but is continuous at a shock. The adjoint solution for the 2D Euler equations is broken into four components. When the base flow field is isentropic, two of the components can be expressed as solutions of the linearised potential flow equations. The third component causes no perturbation to the pressure field and so does not affect the lift and drag on an airfoil. The final component involves perturbations to the stagnation pressure, resulting in an inverse square-root singularity at the stagnation streamline upstream of an airfoil leading edge. This could have significant implications for grid generation and adaptation to achieve more accurate predictions of airfoil lift and drag.

2 Duality and the adjoint formulation

2.1 General theory

If we assume that both the equations and the functional I have been linearised, the discrete approach can be described as a mapping from the original problem,

Determine
$$I = (g, U)$$

given that $A U = f$

into an equivalent dual problem,

Determine
$$I = (V, f)$$

given that $A^T V = g$

The inner product is simply a vector dot product,

$$(V, U) \equiv V^T U,$$

and the equivalence of the two problems is easily proved,

$$(V, f) = (V, A U) = (A^T V, U) = (g, U).$$

Note that the inhomogeneous term f in the discrete equations in the primal problem, enters the functional in the dual problem, and correspondingly the inhomogeneous term g in the dual problem comes from the functional of the primal problem.

Using the analytic approach, the objective is similar, but with linear differential operators instead of matrices, and two additional inner products, one an integral over the domain of the problem,

$$(v,u)_D = \int_D (v,u) \ dV$$

and the other an integral over the boundary of the domain,

$$(v, u)_{\partial D} = \int_{\partial D} (v, u) \ dA$$

With these definitions, the objective in the analytic approach is to convert the primal problem,

Determine
$$I = (g, u)_D + (h, Cu)_{\partial D}$$

given that $Lu = f$ in D
and $Bu = e$ on ∂D .

into an equivalent dual problem,

Determine
$$I = (v, f)_D + (C^*v, e)_{\partial D}$$

given that $L^*v = g$ in D
and $B^*v = h$ on ∂D .

 L^* is the linear p.d.e. which is adjoint to L. B and B^* are boundary condition operators for the primal and dual problems, respectively, and C and C^* are also operators which may be differential; these four operators, and hence also e and h, may have different dimensions on different parts of the boundary (e.g. inflow and outflow parts of the boundary when L correspond to pure convection).

The equivalence of the two forms of the problem is to be proved by showing that

$$(v, f)_D + (C^*v, e)_{\partial D} = (v, Lu)_D + (C^*v, Bu)_{\partial D} = (L^*v, u)_D + (B^*v, Cu)_{\partial D} = (g, u)_D + (h, Cu)_{\partial D}.$$

The first and last steps involve simple substitutions for e, f, g, h, so the critical step is the central one which requires the identity

$$(v, Lu)_D + (C^*v, Bu)_{\partial D} = (L^*v, u)_D + (B^*v, Cu)_{\partial D},$$

to hold for all u and v.

Integrating by parts gives an identity of the form

$$(v, Lu)_D = (L^*v, u)_D + (A_1v, A_2u)_{\partial D},$$

where L^* is the adjoint partial differential operator, and A_1 and A_2 are differential operators on the boundary ∂D . Therefore, what needs to be proved is that given L, B and C, there exists a pair of operators B^* and C^* such that

$$(A_1v, A_2u)_{\partial D} = (B^*v, Cu)_{\partial D} - (C^*v, Bu)_{\partial D}.$$

We now prove that such operators exist (and are unique) for a large class of p.d.e.'s subject to two restrictions.

<u>Restriction 1:</u> We restrict the theory to p.d.e.'s for which the boundary operators B, C, A_1 and A_2 involve only the values of u and v and any of their normal derivatives, so that

$$Bu \equiv Bu$$
$$Cu \equiv Cu$$
$$(A_1v, A_2u) \equiv v^T Au$$

where \boldsymbol{B} and \boldsymbol{C} are rectangular matrices, \boldsymbol{A} is a square matrix, and \boldsymbol{u} and \boldsymbol{v} are vectors composed of \boldsymbol{u} and \boldsymbol{v} , respectively, together with normal derivatives of the appropriate degree (e.g. the 2D convection/diffusion equation requires first derivatives, whereas the 2D Euler equations need none).

Under this restriction, the result to be proved becomes

$$\int_{\partial D} \boldsymbol{v}^T \boldsymbol{A} \boldsymbol{u} - (\boldsymbol{B}^* \boldsymbol{v})^T \boldsymbol{C} \boldsymbol{u} + (\boldsymbol{C}^* \boldsymbol{v})^T \boldsymbol{B} \boldsymbol{u} \ dA = 0.$$

The necessary and sufficient condition for this to be true is that the integrand is zero at all points. This reduces the task to the linear algebra problem of proving the existence and uniqueness of matrices B^* and C^* at each point of the boundary such that

$$\boldsymbol{A} = (\boldsymbol{B}^*)^T \boldsymbol{C} - (\boldsymbol{C}^*)^T \boldsymbol{B}.$$

It is convenient to define matrices T, T^* as

$$T = \left(rac{B}{C}
ight), \quad T^* = \left(rac{-C^*}{B^*}
ight),$$

so that this equation can be re-written as

$$\boldsymbol{A} = (\boldsymbol{T}^*)^T \boldsymbol{T}.$$

We now make the second restriction, considering first the most common case in which A is non-singular.

Restriction 2 (non-singular form): If A is nonsingular, then the matrix T as defined above is also a non-singular square matrix.

If A is non-singular, then under this restriction T is invertible and so T^* is uniquely defined by

$$\boldsymbol{T}^* = (\boldsymbol{T}^{-1})^T \boldsymbol{A}^T.$$

From the definition of T^* , this then uniquely defines B^* and C^* .

If \boldsymbol{A} is singular, then the first step, both in the theoretical development and in practical applications, is to re-express the problem using reduced vectors $\boldsymbol{u}', \boldsymbol{v}'$ whose dimension equals the rank of \boldsymbol{A} , and for which the corresponding reduced square matrix \boldsymbol{A}' is non-singular. This is accomplished using a singular value decomposition of \boldsymbol{A} ,

$$\boldsymbol{A} = \boldsymbol{R}\,\boldsymbol{\Gamma}\,\boldsymbol{L},$$

in which the matrices \boldsymbol{R} and \boldsymbol{L} are each orthogonal (i.e. $\boldsymbol{R}^{-1} = \boldsymbol{R}^T$, $\boldsymbol{L}^{-1} = \boldsymbol{L}^T$) and $\boldsymbol{\Gamma}$ is a diagonal matrix in which the first m diagonal elements are strictly positive and the remainder are zero. We now define \boldsymbol{A}' to be the $m \times m$ principal diagonal sub-matrix of $\boldsymbol{\Gamma}$ so that

$$A = R'A'L',$$

where \mathbf{R}' is the first *m* columns of \mathbf{R} , and \mathbf{L}' is the first *m* rows of \mathbf{L} , and we define the reduced vectors to be

$$\boldsymbol{u}' = \boldsymbol{L}' \boldsymbol{u}, \quad \boldsymbol{v}' = (\boldsymbol{R}')^T \boldsymbol{v}.$$

In order to be able to express the boundary operators Bu, Cu in terms of the reduced vector u', we need to make the restriction that each row of B and C can be expressed as a linear combination of the rows of A, and hence as a linear combination of the rows of L'. This restriction, together with the requirement that the resulting reduced matrices B' and C' satisfy Restriction 2 given above, can be expressed in the following generalised version of Restriction 2.

Restriction 2:

Given that
$$\boldsymbol{A} \in \mathbb{R}^n \times \mathbb{R}^n$$
 and $\left(\frac{\boldsymbol{B}}{\boldsymbol{C}}\right) \in \mathbb{R}^m \times \mathbb{R}^n$,

then
$$m = \operatorname{rank}(\mathbf{A}) = \operatorname{rank}\left(\frac{\mathbf{B}}{C}\right) = \operatorname{rank}\left(\frac{\mathbf{A}}{\frac{\mathbf{B}}{C}}\right)$$

The analysis so far has been concerned with the construction of a dual problem in which the linear functional is equivalent to that of the primal problem. This has been shown to be achievable if the primal p.d.e., its boundary conditions and its linear functional satisfy certain restrictions. It can also be proved that under these conditions the dual problem is well-posed if, and only if, the primal problem is well-posed.

2.2 2D scalar convection/diffusion equation

The 2D scalar convection/diffusion equation in conservative form is

$$Lu \equiv \nabla \cdot (u\boldsymbol{w}) - \nabla^2 u = f,$$

with \boldsymbol{w} being a prescribed convection velocity. Integrating by parts gives

$$\int_{D} v \left(\nabla \cdot (u \boldsymbol{w}) - \nabla^{2} \boldsymbol{u} \right) dA$$

= $\int_{D} u \left(-\boldsymbol{w} \cdot \nabla v - \nabla^{2} \boldsymbol{v} \right) dA$
+ $\int_{\partial D} v \left(u w_{n} - \frac{\partial u}{\partial n} \right) + u \frac{\partial v}{\partial n} ds.$

Here $w_n \equiv \boldsymbol{w} \cdot \boldsymbol{n}$ and $\partial/\partial n \equiv \boldsymbol{n} \cdot \nabla$, with \boldsymbol{n} being an outward pointing normal on the boundary. Thus, the adjoint p.d.e. is

$$L^* v \equiv -\boldsymbol{w} \cdot \nabla v - \nabla^2 v = g,$$

and the extended vectors $\boldsymbol{u}, \boldsymbol{v}$ and boundary matrix \boldsymbol{A} are

$$\boldsymbol{u} = \left(\begin{array}{c} u \\ rac{\partial u}{\partial n} \end{array}
ight), \quad \boldsymbol{v} = \left(\begin{array}{c} v \\ rac{\partial v}{\partial n} \end{array}
ight), \quad \boldsymbol{A} = \left(\begin{array}{c} w_n & -1 \\ 1 & 0 \end{array}
ight).$$

We now consider two different pairs of boundary operators B and C, and in each case apply the theory to construct the corresponding operators B^* and C^* .

Dirichlet b.c.'s

$$Bu \equiv u, \quad Cu \equiv \frac{\partial u}{\partial n}$$

In this case,

$$T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \implies T^* = \begin{pmatrix} w_n & 1 \\ -1 & 0 \end{pmatrix}.$$

Hence,

$$\boldsymbol{B}^* = \begin{pmatrix} -1 & 0 \end{pmatrix}, \qquad \boldsymbol{C}^* = \begin{pmatrix} -w_n & -1 \end{pmatrix},$$

and so

$$B^*v \equiv -v, \qquad C^*v \equiv -w_nv - \frac{\partial v}{\partial n}.$$

Neumann b.c.'s

$$Bu \equiv \frac{\partial u}{\partial n}, \quad Cu \equiv u$$

In this case,

$$oldsymbol{T} = egin{pmatrix} 0 & 1 \ 1 & 0 \end{pmatrix} \implies oldsymbol{T}^* = egin{pmatrix} -1 & 0 \ w_n & 1 \end{pmatrix}.$$

Hence,

$$\boldsymbol{B}^* = \left(\begin{array}{cc} w_n & 1 \end{array} \right), \qquad \boldsymbol{C}^* = \left(\begin{array}{cc} 1 & 0 \end{array} \right),$$

and so

$$B^*v \equiv w_n v + \frac{\partial v}{\partial n}, \qquad C^*v \equiv v.$$

2.3 2D Euler equations

The nonlinear steady-state Euler equations in conservation form are

$$\frac{\partial}{\partial x}F_x(U) + \frac{\partial}{\partial y}F_y(U) = 0,$$

where U is the vector of conservation variables and $F_x(U)$ and $F_y(U)$ are the nonlinear flux functions,

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

Linearising about a given steady-state solution, U(x, y), leads to the equation

$$Lu \equiv \frac{\partial}{\partial x}(A_x u) + \frac{\partial}{\partial y}(A_y u) = f,$$

where u is the linear perturbation, and the spatially varying matrices A_x, A_y are defined by

$$A_x \equiv \left. \frac{\partial F_x}{\partial U} \right|_{U(x,y)}, \quad A_y \equiv \left. \frac{\partial F_y}{\partial U} \right|_{U(x,y)}.$$

In error analysis, the inhomogeneous term f arises from the truncation error in applying the discrete residual operator to the analytic solution.

In a design application, f is zero if u is defined to be the linear change in the flow solution at a point with fixed coordinates (x, y). However, this definition of uleads to difficulties in approximating the boundary conditions on a perturbed surface [9].

The alternative way of formulating the equations for the design application is to define u to be the linear perturbation in the flow solution taking into account a linear perturbation in the coordinates. This follows the approach now used for linearised unsteady flow analysis [14, 15, 16] in preference to the previous discretisations using fixed grids [17, 18].

The starting point for this formulation is the conservative form of the Euler equation using general curvilinear coordinates,

$$\frac{\partial}{\partial\xi} \left(F_x \frac{\partial y}{\partial \eta} - F_y \frac{\partial x}{\partial \eta} \right) + \frac{\partial}{\partial\eta} \left(F_y \frac{\partial x}{\partial \xi} - F_x \frac{\partial y}{\partial \xi} \right) = 0.$$

We now define the perturbed coordinates as

$$x = \xi + \alpha X(\xi, \eta), \quad y = \eta + \alpha Y(\xi, \eta),$$

where α is a design variable. $X(\xi, \eta)$ and $Y(\xi, \eta)$ are smooth functions which match the surface perturbations due to the design variable, so that a point (ξ, η) which is initially on a solid surface remains so as the design variable changes. Linearising with respect to α yields

$$\begin{aligned} \frac{\partial}{\partial \xi} (A_x u) &+ \frac{\partial}{\partial \eta} (A_y u) = -\frac{\partial}{\partial \xi} \left(F_x \frac{\partial Y}{\partial \eta} - F_y \frac{\partial X}{\partial \eta} \right) \\ &- \frac{\partial}{\partial \eta} \left(F_y \frac{\partial X}{\partial \xi} - F_x \frac{\partial Y}{\partial \xi} \right), \end{aligned}$$

where u is now the perturbation in the flow variables for fixed (ξ, η) rather than fixed (x, y), and the fluxes F_x and F_y are based on the unperturbed flow variables.

Switching notation from (ξ, η) back to (x, y) then produces the equation of the form Lu = f as given above. In essence, this treatment is very similar to that used by Jameson for single-block Euler and Navier-Stokes computations [2, 3]. The difference is that in his formulation the solid surface corresponds to part of the coordinate surface $\eta = 0$, whereas in this formulation the solid surface is the original surface defined in Cartesian coordinates. As a consequence, this new formulation can be used with an unstructured grid discretisation for complex geometries. Returning to the linearised equation, integrating by parts over D gives

$$\left(v, \frac{\partial}{\partial x}(A_x u) + \frac{\partial}{\partial y}(A_y u)\right)_D = \left(-A_x^T \frac{\partial v}{\partial x} - A_y^T \frac{\partial v}{\partial y}, u\right)_D + (v, A_n u)_{\partial D},$$

where

$$A_n = n_x A_x + n_y A_y$$

and $n = (n_x, n_y)^T$ is an outward pointing unit normal on the boundary ∂D .

Thus, the adjoint p.d.e. is

$$L^* v \equiv -A_x^T \frac{\partial v}{\partial x} - A_y^T \frac{\partial v}{\partial y} = g.$$

This can be solved through the evolution to steady-state of the equation

$$\frac{\partial v}{\partial t} - A_x^T \frac{\partial v}{\partial x} - A_y^T \frac{\partial v}{\partial y} = g$$

showing that its characteristic behaviour is similar to that of the original unsteady Euler equations, but with the sign of each characteristic velocity reversed so that the characteristic information travels in the opposite direction.

In applying the general theory to construct the adjoint boundary conditions, the vectors \boldsymbol{u} and \boldsymbol{v} are just \boldsymbol{u} and \boldsymbol{v} , and the matrix \boldsymbol{A} is simply A_n . This can be diagonalised to obtain

$$A_n = R\Lambda R^{-1},$$

in which $\Lambda = \text{diag}(\lambda_i)$ is the diagonal matrix of eigenvalues λ_i of A_n . These can be shown to be

$$\lambda_1 = u_n + c, \quad \lambda_2 = \lambda_3 = u_n, \quad \lambda_4 = u_n - c,$$

where c is the local speed of sound and u_n is the normal component of velocity. The columns of the matrix R are then the corresponding eigenvectors of A.

It is convenient to define primal and dual characteristic variables as

$$u_c = R^{-1}u, \quad v_c = R^T v,$$

so that

$$v^T A_n u = v_c^T \Lambda u_c.$$

We now consider different pairs of boundary operators B and C, expressed in terms of equivalent matrices B_c, C_c applied to the characteristic variables. For each pair, we use the theory to construct corresponding matrices B_c^*, C_c^* , applied to the dual characteristic variables, such that

$$\Lambda = (\boldsymbol{T}_c^*)^T \boldsymbol{T}_c$$

characteristic inflow/outflow b.c.'s

At a subsonic outflow, for which $0 < u_n < c$, the characteristic boundary condition is the specification of the value of the sole incoming characteristic variable, u_{c4} . Thus the characteristic boundary condition operator is

$$Bu \equiv u_{c4} \implies \boldsymbol{B}_c = \left(\begin{array}{ccc} 0 & 0 & 0 & 1 \end{array}\right).$$

Because Λ is non-singular, we need T_c to be square and non-singular and so a suitable characteristic functional is

$$Cu \equiv \begin{pmatrix} u_{c1} \\ u_{c2} \\ u_{c3} \end{pmatrix} \implies C_c = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Together, these give

$$oldsymbol{T}_{c} = egin{pmatrix} 0 & 0 & 0 & 1 \ 1 & 0 & 0 & 0 \ 0 & 1 & 0 & 0 \ 0 & 0 & 1 & 0 \end{pmatrix},$$

and so

$$\boldsymbol{T}_{c}^{*} = \left(\Lambda \, \boldsymbol{T}_{c}^{-1}\right)^{T} = \left(\begin{array}{cccc} 0 & 0 & 0 & \lambda_{4} \\ \lambda_{1} & 0 & 0 & 0 \\ 0 & \lambda_{2} & 0 & 0 \\ 0 & 0 & \lambda_{3} & 0 \end{array}\right).$$

Hence, the characteristic matrices for the dual formulation are

$$\boldsymbol{B}_{c}^{*} = \begin{pmatrix} \lambda_{1} & 0 & 0 & 0 \\ 0 & \lambda_{2} & 0 & 0 \\ 0 & 0 & \lambda_{3} & 0 \end{pmatrix},$$

 and

$$oldsymbol{C}_c^*=\left(egin{array}{cccc} 0 & 0 & 0 & -\lambda_4 \end{array}
ight).$$

Because of the reversal of direction of characteristics, each outgoing characteristic of the primal problem corresponds to an incoming characteristic of the dual problem. Therefore, the boundary condition for the dual problem is indeed well-posed. Similarly, at a subsonic inflow the characteristic operators for the primal problem are

$$Bu \equiv \left(egin{array}{c} u_{c2} \ u_{c3} \ u_{c4} \end{array}
ight), \qquad Cu \equiv u_{c1},$$

and the dual operators are

$$B^*v \equiv \lambda_1 v_{c1},$$

 and

$$C^* v \equiv \begin{pmatrix} -\lambda_2 v_{c2} \\ -\lambda_3 v_{c3} \\ -\lambda_4 v_{c4} \end{pmatrix}$$

solid wall

At a solid wall the normal velocity u_n is zero, so there is only one incoming characteristic for both the primal and the dual problems, and the matrices A_n and Λ are of rank 2 instead of 4. The reduced vectors $\boldsymbol{u}', \boldsymbol{v}'$, as described in the general theory, are

$$oldsymbol{u}' = egin{pmatrix} u_{c1} \ u_{c4} \end{pmatrix}, \quad oldsymbol{v}' = egin{pmatrix} v_{c1} \ v_{c4} \end{pmatrix}$$

and the reduced diagonal matrix Λ' is

$$\Lambda' = \left(\begin{array}{c} c & 0\\ 0 & -c \end{array}\right)$$

An important pair of boundary operators for the primal problem are

$$Bu \equiv \widetilde{u}_n = \frac{u_{c1} - u_{c4}}{2\rho c}, \quad Cu \equiv \widetilde{p} = \frac{u_{c1} + u_{c4}}{2},$$

specifying the perturbation to the normal component of velocity as the boundary condition, and using the linearised pressure perturbation in the functional. These are the boundary operators used in optimal design applications.

Expressed in terms of the reduced vector of characteristic variables, these correspond to

$$B'_c = \left(\begin{array}{cc} \frac{1}{2\rho c} & -\frac{1}{2\rho c} \end{array}
ight), \qquad C'_c = \left(\begin{array}{cc} \frac{1}{2} & \frac{1}{2} \end{array}
ight),$$

and so

$$\mathbf{T}_{c}^{\prime} = \begin{pmatrix} \frac{1}{2\rho c} & -\frac{1}{2\rho c} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix},$$
$$\implies \mathbf{T}_{c}^{\prime *} = \left(\Lambda^{\prime} \mathbf{T}_{c}^{\prime - 1}\right)^{T} = \begin{pmatrix} \rho c^{2} & \rho c^{2} \\ c & -c \end{pmatrix},$$

and hence the dual boundary operators are

$$B^* v \equiv c (v_{c1} - v_{c4}), \qquad C^* v \equiv -\rho c^2 (v_{c1} + v_{c4}).$$

Converting back into the original dual variables gives

$$B^* v \equiv \left(\begin{array}{ccc} 0 & n_x & n_y & 0 \end{array} \right) v,$$

$$C^* v \equiv - \left(\begin{array}{ccc} \rho & \rho u_x & \rho u_y & \rho H \end{array} \right) v$$

Thus, if the primal problem has b.c.

$$\widetilde{u}_n = e_1,$$

and the linear functional includes a surface integral of the quantity

$$h_1\widetilde{p}$$

then the dual problem has b.c.

$$n_x v_2 + n_y v_3 = h_1,$$

and its linear functional includes a surface integral of the quantity

$$e_1 \rho(v_1 + u_x v_2 + u_y v_3 + H v_4).$$

2.4 2D thin shear layer Navier-Stokes equations

The nonlinear steady-state Navier-Stokes equations in conservation form appear as

$$\frac{\partial}{\partial x} F_x(U) + \frac{\partial}{\partial y} F_y(U) = \\ \frac{\partial}{\partial x} F_x^v(U, \frac{\partial U}{\partial x}, \frac{\partial U}{\partial y}) + \frac{\partial}{\partial y} F_y^v(U, \frac{\partial U}{\partial x}, \frac{\partial U}{\partial y}),$$

where $F_x^v(U, \frac{\partial U}{\partial x}, \frac{\partial U}{\partial y})$ and $F_y^v(U, \frac{\partial U}{\partial x}, \frac{\partial U}{\partial y})$ are the nonlinear viscous flux functions.

The linearised equations are

$$Lu \equiv \frac{\partial}{\partial x} \left((A_x - A_x^v)u - D_{xx}\frac{\partial u}{\partial x} - D_{xy}\frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left((A_y - A_y^v)u - D_{yx}\frac{\partial u}{\partial x} - D_{yy}\frac{\partial u}{\partial y} \right) = f,$$

where matrices A_x, A_y are as defined before, and the others are defined as

$$\begin{aligned} A_x^v &\equiv \left. \frac{\partial F_x^v}{\partial U} \right|_{U(x,y)}, \quad A_y^v \equiv \left. \frac{\partial F_y^v}{\partial U} \right|_{U(x,y)}, \\ D_{xx} &\equiv \left. \frac{\partial F_x^v}{\partial (\frac{\partial U}{\partial x})} \right|_{U(x,y)}, \quad D_{yx} \equiv \left. \frac{\partial F_y^v}{\partial (\frac{\partial U}{\partial x})} \right|_{U(x,y)}, \\ D_{xy} &\equiv \left. \frac{\partial F_x^v}{\partial (\frac{\partial U}{\partial y})} \right|_{U(x,y)}, \quad D_{yy} \equiv \left. \frac{\partial F_y^v}{\partial (\frac{\partial U}{\partial y})} \right|_{U(x,y)}. \end{aligned}$$

As with the Euler equations, the inhomogeneous term f corresponds to the truncation error in error analysis, and the result of a linear perturbation to the coordinates in a design application.

Integrating by parts over domain D gives

$$\left(v, \frac{\partial}{\partial x} \left((A_x - A_x^v)u - D_{xx}\frac{\partial u}{\partial x} - D_{xy}\frac{\partial u}{\partial y} \right) \right)_D$$

$$+ \left(v, \frac{\partial}{\partial y} \left((A_y - A_y^v)u - D_{yx}\frac{\partial u}{\partial x} - D_{yy}\frac{\partial u}{\partial y} \right) \right)_D$$

$$= \left(- (A_x - A_x^v)^T \frac{\partial v}{\partial x} - \frac{\partial}{\partial x} \left(D_{xx}^T \frac{\partial v}{\partial x} + D_{yx}^T \frac{\partial v}{\partial y} \right), u \right)_D$$

$$+ \left(- (A_y - A_y^v)^T \frac{\partial v}{\partial y} - \frac{\partial}{\partial y} \left(D_{xy}^T \frac{\partial v}{\partial x} + D_{yy}^T \frac{\partial v}{\partial y} \right), u \right)_D$$

$$+ \left(v, n_x \left((A_x - A_x^v)u - D_{xx}\frac{\partial u}{\partial x} - D_{xy}\frac{\partial u}{\partial y} \right) \right)_{\partial D}$$

$$+ \left(v, n_y \left((A_y - A_y^v)u - D_{yx}\frac{\partial u}{\partial x} - D_{yy}\frac{\partial u}{\partial y} \right) \right)_{\partial D}$$

$$+ \left(\frac{\partial v}{\partial x}, (n_x D_{xx} + n_y D_{yx})u \right)_{\partial D}$$

$$+ \left(\frac{\partial v}{\partial y}, (n_x D_{xy} + n_y D_{yy})u \right)_{\partial D} ,$$

where $(n_x, n_y)^T$ is again an outward pointing unit normal on the boundary ∂D .

The adjoint p.d.e. is therefore

$$\begin{split} L^* v &\equiv -(A_x - A_x^v)^T \frac{\partial v}{\partial x} - (A_y - A_y^v)^T \frac{\partial v}{\partial y} \\ &- \frac{\partial}{\partial x} \left(D_{xx}^T \frac{\partial v}{\partial x} + D_{yx}^T \frac{\partial v}{\partial y} \right) \\ &- \frac{\partial}{\partial y} \left(D_{xy}^T \frac{\partial v}{\partial x} + D_{yy}^T \frac{\partial v}{\partial y} \right) = g, \end{split}$$

which can be solved through the evolution to steadystate of the equation

$$\frac{\partial v}{\partial t} - (A_x - A_x^v)^T \frac{\partial v}{\partial x} - (A_y - A_y^v)^T \frac{\partial v}{\partial y} - \frac{\partial}{\partial x} \left(D_{xx}^T \frac{\partial v}{\partial x} + D_{yx}^T \frac{\partial v}{\partial y} \right) - \frac{\partial}{\partial y} \left(D_{xx}^T \frac{\partial v}{\partial x} + D_{yx}^T \frac{\partial v}{\partial y} \right) = g.$$

We now consider the formulation of adjoint boundary conditions at a solid wall, which for convenience is initially assumed to be locally aligned with the x-axis so that the outward normal from the fluid is $(0\ 1)^T$. Because the viscous fluxes involve derivatives of temperature and the two velocity components, it is helpful to switch to new variables, $u_p \equiv (\tilde{\rho} \ \tilde{u}_x \ \tilde{u}_y \ \tilde{T})^T$, in which $\tilde{\rho}$ and \tilde{T} are the linear perturbations in density and temperature, respectively, and \tilde{u}_x and \tilde{u}_y are the perturbations to the components of velocity in the two coordinate directions. The linearised conservation variables u can be related to the new variables u_p by

$$u = Su_p,$$

The corresponding extended vectors \boldsymbol{u}_p and \boldsymbol{v}_p are defined by

$$\boldsymbol{u}_{p} = \begin{pmatrix} u_{p} \\ \frac{\partial u_{p}}{\partial n} \end{pmatrix} = \begin{pmatrix} S^{-1}u \\ \frac{\partial}{\partial n}(S^{-1}u) \end{pmatrix}, \qquad \boldsymbol{v}_{p} = \begin{pmatrix} S^{T}v \\ S^{T}\frac{\partial v}{\partial n} \end{pmatrix}.$$

Making a high Reynolds number thin-shear-layer approximation in which streamwise viscous derivatives are neglected, and ignoring the weak temperature dependence of the viscosity and thermal conductivity, the boundary term arising from the integration by parts can eventually be written as $v_p^T A_p u_p$ where A_p is

Here τ_{xy} and τ_{yy} are the x and y components of the shear stress acting on the solid wall, μ, λ and k are the usual coefficients of viscosity and thermal conductivity, R is the gas constant, and c_v is the specific heat at constant volume.

The matrix A_p is of rank 6 since each of its rows can

be expressed as a combination of the rows

(0	1	0	0	0	0	0	0)
(0	0	1	0	0	0	0	0)
(0	0	0	1	0	0	0	0)
(0	0	0	0	0	$-\mu$	0	0)
(RT	0	0	ho R	0	0	$-(2\mu + \lambda)$	0)
(0	0	0	0	0	0	0	-k)

which correspond to perturbations in the two velocity components, the temperature, the two components of surface force, and the surface heat flux, respectively.

The Navier-Stokes equations require a total of three boundary conditions at a solid wall. Two of these come from the no-slip condition requiring both components of the velocity to be zero. The third involves the temperature, specifying either its value or its normal derivative.

Specified temperature

If the temperature is specified, the boundary operator matrix \boldsymbol{B}_p has the form

$$\boldsymbol{B}_p = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

A valid choice for the boundary operator C is to select the two components of surface force and the heat flux, giving

$$\boldsymbol{C}_p = \left(\begin{array}{cccccccc} 0 & 0 & 0 & 0 & -\mu & 0 & 0 \\ RT & 0 & 0 & \rho R & 0 & 0 & -(2\,\mu + \lambda) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -k \end{array} \right).$$

The rows of B_p and C_p are then linearly independent, and together form a complete basis for the rows of A_p , which can be factored to obtain the following boundary operator matrices for the adjoint formulation,

$$\boldsymbol{B}_{p}^{*} = \left(\begin{array}{cccccc} 0 & \frac{1}{\rho} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\rho} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\rho c_{v}} & 0 & 0 & 0 & 0 \end{array}\right),$$

 and

$$\begin{split} \boldsymbol{C}_{p}^{*} &= \\ & \begin{pmatrix} 0 & 0 & 0 & \frac{\tau_{xy}}{\rho c_{v}} & 0 & -\frac{\mu}{\rho} & 0 & 0 \\ -\rho & 0 & 0 & -(\gamma - 1)T + \frac{\tau_{yy}}{\rho c_{v}} & 0 & 0 & -\frac{2\mu + \lambda}{\rho} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{k}{\rho c_{v}} \end{pmatrix} \end{split}$$

Converting back into the original variables, the adjoint boundary operators are

$$B^* v \equiv \left(\begin{array}{rrrr} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right) v,$$

 and

$$C^* v \equiv \begin{pmatrix} 0 & 0 & 0 & \tau_{xy} \\ -\rho & 0 & 0 & -\rho H + \tau_{yy} \\ 0 & 0 & 0 & 0 \end{pmatrix} v \\ - \begin{pmatrix} 0 & \mu & 0 & 0 \\ 0 & 0 & 2\mu + \lambda & 0 \\ 0 & 0 & 0 & k \end{pmatrix} \frac{\partial v}{\partial y}.$$

In the more general case in which the x-axis is not aligned with the surface, the linear functional can be taken to be a surface integral of

$$h^T C u \equiv h_1 \widetilde{\sigma}_{xn} + h_2 \widetilde{\sigma}_{yn} + h_3 \widetilde{q}_n,$$

where $\tilde{\sigma}_{xn}$ and $\tilde{\sigma}_{yn}$ are the linear perturbations to the two components of the force exerted by the fluid on the surface (including both the pressure and shear stress terms), and \tilde{q}_n is the perturbation heat flux into the surface. The boundary conditions for the adjoint equations are then

$$egin{array}{rcl} v_2 &=& h_1, \ v_3 &=& h_2, \ v_4 &=& h_3. \end{array}$$

The boundary data for the primal problem is typically

$$\begin{aligned} \widetilde{u}_x &= 0, \\ \widetilde{u}_y &= 0, \\ \widetilde{T} &= e_3, \end{aligned}$$

so that the surface contribution to the linear functional in the dual formulation is

$$e^T C^* v \equiv -k \, e_3 \, \frac{\partial v_4}{\partial n}$$

This simple form for the adjoint boundary conditions and linear functional can be easily verified by using integration by parts to confirm the identity

$$(v,f)_D + (C^*v,e)_{\partial D} = (g,u)_D + (h,Cu)_{\partial D}.$$

The advantage of deriving it by the more formal procedure above is that it proves the limited options for the operator Cu in the primal functional. For example, one of the rows of Cu can be $\frac{\partial T}{\partial n}$, but it could not be $\frac{\partial p}{\partial n}$.

Specified heat flux

Reverting to the simplifying assumption that the boundary is aligned with the x-axis, the boundary operator matrix \boldsymbol{B}_p in the case of specified heat flux is

and a valid choice for the boundary operator C_p is to select the the two components of surface force and the temperature, giving

$$\boldsymbol{C}_{p} = \begin{pmatrix} 0 & 0 & 0 & 0 & -\mu & 0 & 0 \\ RT & 0 & 0 & \rho R & 0 & 0 & -(2\mu + \lambda) & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

The only difference from the previous case is the interchange of the last lines in B_p and C_p . Following the same procedure, the adjoint boundary operators are found to be

 and

$$C^* v \equiv \begin{pmatrix} 0 & 0 & 0 & \tau_{xy} \\ -\rho & 0 & 0 & -\rho H + \tau_{yy} \\ 0 & 0 & 0 & -1 \end{pmatrix} v \\ - \begin{pmatrix} 0 & \mu & 0 & 0 \\ 0 & 0 & 2\mu + \lambda & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \frac{\partial v}{\partial y}.$$

Switching back to general coordinates, with a linear functional which is a surface integral of

$$h^T C u \equiv h_1 \widetilde{\sigma}_{xn} + h_2 \widetilde{\sigma}_{yn} + h_3 \widetilde{T},$$

the boundary conditions for the adjoint equations are

$$v_2 = h_1,$$

$$v_3 = h_2,$$

$$k \frac{\partial v_4}{\partial n} = h_3.$$

The boundary data for the primal problem is

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$$\begin{aligned} \widetilde{u}_x &= 0, \\ \widetilde{u}_y &= 0, \\ \widetilde{q}_n &= e_3, \end{aligned}$$

and the surface contribution to the linear functional in the dual formulation is

$$e^T C^* v \equiv -e_3 v_4.$$

3 Green's functions and adjoint solutions

In this section the aim is to find the Green's function $G(x, \xi)$ such that the solution of the inhomogeneous linearised Euler equations,

$$Lu = f$$

subject to homogeneous b.c.'s can be expressed as

$$u(\boldsymbol{x}) = \int_D G(\boldsymbol{x}, \boldsymbol{\xi}) f(\boldsymbol{\xi}) d\boldsymbol{\xi}.$$

 $G(\boldsymbol{x}, \boldsymbol{\xi})$ is a matrix function whose dimension d is equal to 3 for the quasi-1D Euler equations, and 4 for the 2D Euler equations. Given d vector functions $f_n(\boldsymbol{\xi})$, let the associated functions $u_n(\boldsymbol{x}, \boldsymbol{\xi})$ be the solution to

$$Lu_n(\boldsymbol{x},\boldsymbol{\xi}) = f_n(\boldsymbol{\xi})\,\delta(\boldsymbol{x}-\boldsymbol{\xi}),$$

where $\delta(\boldsymbol{x} - \boldsymbol{\xi})$ is the Dirac delta function, and the boundary conditions are again homogeneous.

If the vector functions f_n are linearly independent at each point $\boldsymbol{\xi}$, then by linear superposition the Green's function can be expressed as the following combination of two matrices whose columns are the vectors u_n and f_n ,

$$G(\boldsymbol{x},\boldsymbol{\xi}) = \left(\left. u_1 \right| u_2 \right| \dots \left| u_d \right. \right) \left(\left. f_1 \right| f_2 \left| \dots \right| f_d \right. \right)^{-1}$$

In addition, if $I_n(\boldsymbol{\xi})$ is the value of the linear functional corresponding to $u_n(\boldsymbol{x}, \boldsymbol{\xi})$ then, by definition,

$$I_n(\boldsymbol{\xi}) = (v(x), \ f_n(\boldsymbol{\xi}) \ \delta(\boldsymbol{x} - \boldsymbol{\xi}))_D = v^T(\boldsymbol{\xi}) f_n(\boldsymbol{\xi}) \quad (1)$$

and hence

$$v^{T}(\boldsymbol{\xi}) = \left(\left| I_{1} \right| | I_{2} \right| \dots \left| I_{d} \right| \right) \left(\left| f_{1} \right| | f_{2} \right| \dots \left| f_{d} \right| \right)^{-1}$$

In the analyses below for the quasi-1D and 2D Euler equations, the approach in each case is to construct functions $f_n(\boldsymbol{\xi})$ which produce solutions $u_n(\boldsymbol{x}, \boldsymbol{\xi})$ of a simple form. The objective is to gain insight into the nature of the Green's function and the adjoint solution, in particular looking for singularities and discontinuities in the adjoint variables. Furthermore, given a computed adjoint solution \boldsymbol{v} and a set of perturbation vectors $f_n(\boldsymbol{\xi})$, it is then possible to evaluate the corresponding linear functionals $I_n(\boldsymbol{\xi})$ using Equation (1). This provides a means of verifying a number of the adjoint solution properties derived in the following section.

3.1 Quasi-1D Euler equations

The nonlinear quasi-1D Euler equations in conservation form are

$$\frac{d}{dx}(hF) - \frac{dh}{dx}P = 0,$$

where h is the streamtube height and

$$F = \begin{pmatrix} \rho q \\ \rho q^2 + p \\ \rho q H \end{pmatrix}, \quad P = \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix},$$

with q being the velocity and the other variables are as defined previously.

The linearised equations are then

$$Lu \equiv \frac{d}{dx}(hAu) - \frac{dh}{dx}Bu = f,$$

where

$$A = \frac{\partial F}{\partial U}, \quad B = \frac{\partial P}{\partial U}.$$

3.1.1 Singularity at a sonic throat

The first case to be considered is a convergingdiverging duct with sonic conditions at the throat at x = 0, subsonic flow upstream of it, and supersonic flow downstream. The inflow boundary conditions at x = -1 are specified stagnation enthalpy H and stagnation pressure p_o , and there are no outflow boundary conditions at x = 1.

The nonlinear equations ensure that mass flux, stagnation enthalpy and stagnation pressure all remain constant along the duct. Likewise, if $f(x) = f_n(\xi)\delta(x-\xi)$ then the linear perturbation in mass flux, stagnation enthalpy and stagnation pressure will be constant for $x < \xi$ and $x > \xi$. This observation, together with the fact that the Mach number remains equal to unity at the throat, leads to the following solutions u_n and functions f_n .

change in mass flow at fixed H, p_o

The mass flow is equal to mh where $m = \rho q$. The solution to be constructed corresponds to a unit change in mass flow at the point $x = \xi$, keeping H, p_o unchanged. Because H, p_o are unchanged and the throat remains sonic, the mass flow through the throat must remain fixed. Hence, if $\xi < 0$, the mass flow upstream of $x = \xi$ is reduced by a unit amount, whereas if $\xi > 0$, it is the mass flow downstream of $x = \xi$ which is increased by a unit amount.

Defining $m = \rho q$, and using the Heaviside function $\mathcal{H}(x)$, this leads to the following function u_1

$$u_1(x,\xi) = \begin{cases} \left. -\frac{1}{h(x)} \mathcal{H}(\xi - x) \left. \frac{\partial U}{\partial m}(x) \right|_{H,p_o}, \ \xi < 0 \\ \left. \frac{1}{h(x)} \mathcal{H}(x - \xi) \left. \frac{\partial U}{\partial m}(x) \right|_{H,p_o}, \ \xi > 0 \end{cases}$$

which is a solution to the linearised flow equations when $f(x) = f_1(\xi)\delta(x-\xi)$ and

$$f_1(\xi) = \left. \frac{\partial F}{\partial m}(\xi) \right|_{H,p_o \text{ fixed}}$$

Here, as in several of the cases that follow, the form of the perturbation source vector f_n required to produce a prescribed solution perturbation u_n , is determined by analogy to a Rankine-Hugoniot jump condition expressed in terms of the nonlinear solution and flux vectors U and F.

If the linear functional is

$$I = \int_{-1}^{1} \widetilde{p} \, dx$$

where \tilde{p} is the linearised perturbation to the pressure, then

$$u_1(x,\xi) = \begin{cases} -\int_{-1}^{\xi} \frac{1}{h(x)} \left. \frac{\partial p}{\partial m}(x) \right|_{H,p_o} dx, \ \xi < 0\\ \\ \int_{\xi}^{1} \frac{1}{h(x)} \left. \frac{\partial p}{\partial m}(x) \right|_{H,p_o} dx, \ \xi > 0 \end{cases}$$

Since

$$\frac{\partial p}{\partial m} \sim \frac{1}{x}, \quad \text{as} \quad x \to 0,$$

it follows that

$$I_1(\xi) \sim \log(\xi), \quad \text{as} \quad \xi \to 0.$$

and thus there is a logarithmic singularity in the adjoint variables at the sonic throat.

change in H at fixed p_o, M

In this case, the stagnation enthalpy downstream of $x = \xi$ is perturbed by a unit amount, in the linearised sense. Keeping the Mach number unchanged ensures the perturbation in mass flux is constant.

The solution $u_2(x,\xi)$ is given by

$$u_2(x,\xi) = \mathcal{H}(x-\xi) \left. \frac{\partial U}{\partial H}(x) \right|_{p_o,M}$$
 fixed

corresponding to

$$f_2(\xi) = h(\xi) \left. \frac{\partial F}{\partial H}(x) \right|_{p_o, M \text{ fixed}}.$$

Since p_o and M are fixed, there is no perturbation to the pressure and hence $I_2(\xi) = 0$.

change in p_o at fixed H, M

The final case perturbs the stagnation pressure by a unit amount downstream of $x = \xi$, keeping the stagnation enthalpy and Mach number fixed. This again implies a uniform perturbation to the downstream mass flux and so the linearised equations are satisfied by

$$u_3(x,\xi) = \mathcal{H}(x-\xi) \left. \frac{\partial U}{\partial p_o}(x) \right|_{H,M}$$
 fixed

with

$$f_3(\xi) = h(\xi) \left. \frac{\partial F}{\partial p_o}(x) \right|_{H,M}$$
 fixed

The corresponding linearised functional is

$$I_3(\xi) = \int_{\xi}^1 \left. \frac{\partial p}{\partial p_o}(x) \right|_{H,M} dx = \int_{\xi}^1 \frac{p}{p_o} dx,$$

which does not exhibit a singularity at the throat.

3.1.2 Continuity at a shock

Suppose now that we have a diverging duct with a shock at x = 0. The nonlinear Rankine-Hugoniot equations prescribe a zero jump in the flux F,

$$[F]_{0^{-}}^{0^{+}} = 0.$$

If the shock is displaced to $x = x_s$ then this becomes

$$[F]_{x_{s}^{-}}^{x_{s}^{+}} = 0.$$

Linearising about the base solution at x = 0 gives the following linearised Rankine-Hugoniot equations,

$$\left[Au + x_s \frac{dF}{dx}\right]_{0^-}^{0^+} = 0.$$

If the linear equations have source term $f(\xi) \, \delta(x-\xi)$ at a point ξ just upstream of the shock, the jump condition at ξ is

$$[Au]_{\xi^-}^{\xi^+} = f(\xi).$$

In the limit as $\xi \to 0$, this can be combined with the Rankine-Hugoniot jump to give

$$\left[Au + x_s \frac{dF}{dx}\right]_{0^-}^{0^+} = f(\xi).$$

Repeating this argument for $\xi > 0$, $\xi \to 0$ results in the same expression. Therefore, since the jump equations are the same in the two limits, so too are the Green's functions. i.e. $G(x,\xi)$ is continuous in ξ at the shock, even though it is discontinuous in x. A consequence is that the adjoint solution $v(\xi)$ is continuous at the shock.

Further analysis reveals the gradient of $v(\xi)$ is discontinuous at the shock.

3.2 2D Euler equations

Here we consider flow around an isolated airfoil with subsonic freestream conditions. The behaviour of the Green's function and the adjoint variables is determined through the analysis of the response to four linearly independent source terms.

mass source at fixed p_o, H

As with the quasi-1D Euler equations, the first source to be considered is a unit mass source injecting fluid with the local values of stagnation pressure and enthalpy. By considering a small control volume surrounding the point $\boldsymbol{\xi}$ at which the mass is being injected, it can be determined that the relevant source term is $f_1(\boldsymbol{\xi}) \,\delta(\boldsymbol{x} - \boldsymbol{\xi})$ where

$$f_1(\boldsymbol{\xi}) = \begin{pmatrix} 1 \\ u_x \\ u_y \\ H \end{pmatrix}.$$



Figure 1: Global domain of influence due to mass injection in the supersonic region.

If the entire flow field is subsonic, the response $u_1(x, \xi)$ to this source can be obtained from the linearised potential flow equations. In the limit as ξ approaches the surface of the airfoil, the local behaviour can be analysed by using a Prandtl-Glauert transformation to relate the flow field to that of an incompressible flow field with a point mass source. This analysis reveals that there is no singularity as ξ approaches the surface. Similarly there is no singularity as ξ crosses the stagnation streamline either upstream or downstream of the airfoil.

If the flow field is transonic, it raises the question of whether there is a singularity at either the sonic line or a shock. At a shock, the quasi-1D analysis can be extended to prove that the Green's function and the adjoint variables are continuous as $\boldsymbol{\xi}$ crosses the shock, although there is a discontinuity in the gradient of the adjoint variables. Hence, in particular, $u_1(\boldsymbol{x}, \boldsymbol{\xi})$ is continuous with respect to $\boldsymbol{\xi}$ across the shock.

The behaviour at the sonic line is very hard to analyse, but it appears that in general there is no singularity, in contrast to the logarithmic singularity for the quasi-1D equations. The reason for this is that in 2D flows the sonic line is almost never perpendicular to the local streamlines. As illustrated in Figure 1, this is important because when mass is injected into the flow on the supersonic side of the sonic line, the influence of this extends along the Mach lines coming out of $\boldsymbol{\xi}$. If the sonic line is not perpendicular to the streamlines, the Mach lines reach the sonic line and the influence then extends throughout the elliptic region and hence to the whole supersonic region. This lateral pressure relief mechanism prevents the singular response exhibited in the quasi-1D case, and ensures that $u_1(\boldsymbol{x},\boldsymbol{\xi})$ is continuous with respect to $\boldsymbol{\xi}$ as $\boldsymbol{\xi}$ crosses the sonic line. Consequently, the response of a linearised functional, such as the perturbation to the lift or drag, will also be continuous.

normal force

The second source term corresponds to an applied force in the direction normal to the local flow,

$$f_2(\boldsymbol{\xi}) = egin{pmatrix} 0 \ -
ho u_y \
ho u_x \ 0 \end{pmatrix}.$$

If the flow is subsonic, this can again be represented by the linearised potential flow equations, and in this case the point force will correspond to a vortex of unit strength. In the limit as the vortex approaches the surface of the airfoil, a Prandtl-Glauert transformation to an incompressible flow field can again be used, and this time it reveals that $u_2(x, \boldsymbol{\xi}) \to 0$ except in the immediate vicinity of $\boldsymbol{x} = \boldsymbol{\xi}$, and that the force exerted on the surface is $\rho q(\boldsymbol{\xi})$, where $q^2 = u_x^2 + u_y^2$. Hence, if the linear functional is $(\tilde{p}, h)_{\partial D}$, then the linear functional due to $u_2(\boldsymbol{x}, \boldsymbol{\xi})$ is

$$I_2(\boldsymbol{\xi}) = \left.
ho qh \right|_{\boldsymbol{x}=\boldsymbol{\xi}}$$
 .

Since $I_2(\boldsymbol{\xi}) = v^T(\boldsymbol{\xi}) f_2(\boldsymbol{\xi})$ it follows therefore that

$$n_x v_2 + n_y v_3 = h,$$

which is the adjoint b.c. derived earlier.

As with the point mass source, the response to this point force is continuous as $\boldsymbol{\xi}$ crosses the stagnation streamline, the sonic line, and any shocks.

change in H at fixed p_o, p

The third source term is essentially the same as the second of those for the quasi-1D equations. Consider an infinitesimal streamtube with mass flux ϵ passing through $\boldsymbol{\xi}$. The fluid in the streamtube downstream of $\boldsymbol{\xi}$ is subjected to a unit linearised perturbation to the stagnation enthalpy H, keeping fixed the stagnation pressure p_o , the static pressure p and the flow angle α . This perturbed streamtube satisfies the linearised Euler equations, with the constant pressure being important to maintain pressure equilibrium with neighbouring streamtubes.

Using curvilinear streamline coordinates in which s is the distance along the streamline downstream of $\boldsymbol{\xi}$ and n is the coordinate perpendicular to the streamline, and dividing by ϵ to re-normalise, the linear solution $u_3(\boldsymbol{x}, \boldsymbol{\xi})$ is

$$u_3(\boldsymbol{x}, \boldsymbol{\xi}) = \mathcal{H}(s)\delta(n) rac{1}{
ho q} \left. rac{\partial U}{\partial H}(\boldsymbol{x})
ight|_{p_o, p, lpha} ext{ fixed }.$$



Figure 2: Orientation of Heaviside step and Dirac delta functions used to describe the perturbation to a streamtube.

The term $\frac{1}{\rho q}$ reflects the fact that the width of the streamtube is inversely proportional to the mass flow per unit area. The orientation of the Heaviside step function and Dirac delta function with respect to the streamtube is illustrated in Fig. 2, where the influence of the perturbation source is depicted as a discontinuity at $\boldsymbol{\xi}$.

The source term that creates this solution is $f_3(\boldsymbol{\xi}) \,\delta(\boldsymbol{x} - \boldsymbol{\xi})$, where

$$f_3(\boldsymbol{\xi}) = \frac{1}{\rho q} \left. \frac{\partial}{\partial H} (n_x F_x + n_y F_y) \right|_{p_o, p, \alpha \text{ fixed}},$$

and $(n_x, n_y)^T$ is the unit vector in the flow direction at $\boldsymbol{\xi}$. After some algebra, this reduces to

$$f_3(\boldsymbol{\xi}) = \begin{pmatrix} -\frac{1}{2H} \\ 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$$

If the linearised functional is of the form $(\tilde{p}, h)_{\partial D}$, then since the static pressure is unaffected by this source term $I_3(\boldsymbol{\xi})$ is identically zero.

change in p_o at fixed H, p

The fourth source term is similar to the previous, but involves a perturbation to the stagnation pressure instead of the stagnation enthalpy. Therefore the source term is $f_4(\boldsymbol{\xi}) \,\delta(\boldsymbol{x} - \boldsymbol{\xi})$ where

$$f_4(\boldsymbol{\xi}) = \frac{1}{\rho q} \left. \frac{\partial}{\partial p_o} (n_x F_x + n_y F_y) \right|_{H,p,\alpha \text{ fixed}}.$$

This may be evaluated to give

$$f_4(m{\xi}) = egin{pmatrix} rac{1}{p_0} (rac{\gamma-1}{\gamma} + rac{1}{\gamma M^2}) \ rac{u_x}{p_0} (rac{\gamma-1}{\gamma} + rac{2}{\gamma M^2}) \ rac{u_y}{p_0} (rac{\gamma-1}{\gamma} + rac{2}{\gamma M^2}) \ rac{\mu_y}{p_0} (rac{\gamma-1}{\gamma} + rac{2}{\gamma M^2}) \ rac{H}{p_0} (rac{\gamma-1}{\gamma} + rac{1}{\gamma M^2}) \end{pmatrix}.$$

The perturbation this produces in the streamtube downstream of $\boldsymbol{\xi}$ is

$$\left. \mathcal{H}(s)\delta(n) rac{1}{
ho q} \left. rac{\partial U}{\partial p_o}(oldsymbol{x})
ight|_{H,p,lpha ext{ fixed}}$$

However, this is not the full form of the solution u_4 because it produces a non-uniform perturbation to the mass flux through the streamtube. Note that this is in contrast to the third source term for the quasi-1D analysis for which the perturbation was at constant Mach number, not constant pressure, and so there was a uniform perturbation to the mass flux. However, in the 2D case, the pressure must remain fixed to maintain pressure equilibrium with neighbouring streamtubes.

The linearised mass flux perturbation is given by

$$\widetilde{m} = \frac{1}{\rho q} \left. \frac{\partial(\rho q)}{\partial p_o}(x) \right|_{H,p \text{ fixed}}$$

Thus, at a point $\mathbf{x}'(s)$ on the streamline a distance s downstream of $\boldsymbol{\xi}$, there is a mass transpiration of strength $-d\tilde{m}/ds$. The response to this is given by the function $u_1(\mathbf{x}, \mathbf{x}'(s))$ and hence the full solution $u_4(\mathbf{x}, \boldsymbol{\xi})$ is

$$u_4(\boldsymbol{x},\boldsymbol{\xi}) = \mathcal{H}(s)\delta(n)\frac{1}{\rho q} \left.\frac{\partial U}{\partial p_o}(\boldsymbol{x})\right|_{H,p,\alpha} \\ - \int_0^\infty \frac{d\widetilde{m}}{ds} u_1(\boldsymbol{x},\boldsymbol{x}'(s)) \, ds.$$

The corresponding linearised functional is then

$$I_4(\boldsymbol{\xi}) = -\int_0^\infty rac{d\widetilde{m}}{ds} I_1(\boldsymbol{x}'(s)) \, ds.$$

This solution has an interesting behaviour near the stagnation streamline upstream of the airfoil. As $\boldsymbol{\xi}$ crosses the stagnation streamline, the integral switches abruptly from being along a streamline passing over the suction surface of the airfoil, to one passing over the pressure surface. Thus, at the very least, one would expect a discontinuity in both $u_4(\boldsymbol{x}, \boldsymbol{\xi})$ and $I_4(\boldsymbol{\xi})$ as $\boldsymbol{\xi}$ crosses the stagnation streamline.

In fact, there appears to be a singularity at the stagnation streamline, with $I_4(\boldsymbol{\xi})$ being proportional to $n^{-1/2}$ where *n* is the distance from the stagnation streamline. To show this it is necessary first to integrate by parts to obtain

$$I_4(\boldsymbol{\xi}) = -\left[\widetilde{m}(s)I_1(\boldsymbol{x}'(s))\right]_0^\infty + \int_0^\infty \widetilde{m}\,\frac{dI_1}{ds}\,ds$$

In incompressible flow,

$$p_o = p + \frac{1}{2}\rho q^2$$

and hence

$$\widetilde{m} = rac{1}{
ho q} \left. rac{\partial(
ho q)}{\partial p_o}(x)
ight|_{H,p} = rac{1}{
ho q^2}$$

Also, the asymptotic form of the streamfunction for the incompressible flow at the leading edge stagnation point is

$$\psi = cxy,$$

from which it follows that the flow speed is given by

$$q = |c|r, \quad r^2 = x^2 + y^2,$$

and that the minimum distance from a particular streamline to the stagnation point is

$$r_{min} = \left|\frac{2\psi}{c}\right|^{\frac{1}{2}}.$$

Thus, $\widetilde{m} = O(r^{-2})$ and $\frac{dI_1}{ds} = O(1)$, and so, integrating along a streamline,

$$I_4(\boldsymbol{\xi}) \sim r_{min}^{-1} \sim |\psi|^{-\frac{1}{2}} \sim |n|^{-\frac{1}{2}}.$$

If there is a stagnation point at the trailing edge of the airfoil, a similar analysis will apply in the limit as $\boldsymbol{\xi}$ approaches the airfoil surface, producing a singularity whose exponent will depend on the trailing edge wedge angle.

Having determined the form of the four source perturbations, it is now possible to verify some of the derived adjoint solution properties by examining an adjoint solution generated using Jameson's 2D Euler design code SYN82 [2]. The linear functional for this calculations was of the form $(h, \tilde{p})_{\partial D}$, and the individual contributions of the four source perturbations to this functional are depicted in the contour plots of Fig. 3.

Figure 3a) shows that $I_1(\boldsymbol{\xi})$ is continuous with a steep gradient near the leading edge just downstream of the sonic line. A discontinuity in the gradient of I_1 is noticeable at the shock, but is more clearly seen in the surface line plot in Fig. 4. Figure 3b) confirms that $I_2(\boldsymbol{\xi})$ is also continuous, with a discontinuous gradient at the shock.

Figure 3c), which is generated using the same contour increment as the other three figures, confirms that I_3 is zero to within the limits of numerical truncation error.

Figure 3d) reveals a rapid variation in $I_4(\boldsymbol{\xi})$ as $\boldsymbol{\xi}$ crosses the incoming stagnation streamline. Figure 5



Figure 4: Surface plot of I_1 resulting from a point mass source.



Figure 5: Plot of I_4 along a line crossing the stagnation streamline upstream of the airfoil as indicated in Fig. 3d.

shows the variation along the line upstream of the airfoil indicated in Figure 3d). This confirms a combination of a step change in I_4 plus some form of apparent singularity. However, a detailed grid convergence study would need to be performed to verify the predicted inverse square-root nature of this singularity.

4 Conclusions

In this paper we have considered a number of mathematical aspects of the formulation and solution of the adjoint equations for compressible flow. The boundary condition analysis has shown that at solid walls the linear functional must be a function of the linearised



3a: I_1 due to point mass source.

3b: I_2 due to point force.





3c: I_3 due to stagnation enthalpy perturbation.

3d: $I_4\,$ due to stagnation pressure perturbation.

Figure 3: Contribution of source terms to the linear functional. Contour increment is 0.04 in all cases.

pressure perturbation in the case of inviscid flow, and a function of the normal and tangential forces and some combination of the temperature and heat flux in the case of viscous flows. No other choices lead to a well-posed problem.

The construction of Green's functions for the Euler equations has revealed the behaviour of the adjoint variables. For a quasi-1D duct there is a logarithmic singularity at a sonic throat, whereas at a shock the adjoint variables are continuous but the gradient is not. In 2D, the Green's function and adjoint variables are broken into four components. Two of these correspond to potential flow perturbations for which the adjoint solutions are smooth; this is confirmed by numerical results which also reveal strong gradients near the sonic line. The third component involves perturbations to the stagnation enthalpy and produces no perturbation to the pressure and hence the associated linear functional is zero; this is confirmed by the numerical results. The fourth component involves perturbations to the stagnation pressure. The analysis reveals the existence of an inverse square-root singularity crossing the incoming stagnation streamline, but further numerical investigation is needed to confirm this.

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