An Adjoint Method for the Calculation of Non-Collocated Sensitivities in Supersonic Flow

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Abstract

This paper presents an adjoint method for the calculation of non-collocated sensitivities in supersonic flow. The goal is to develop a set of discrete adjoint equations and their corresponding boundary conditions in order to quantify the influence of geometry modifications on the pressure distribution at an arbitrary location within the domain of interest. First, this paper presents the complete formulation and discretization of the discrete adjoint equations. The special treatment of the adjoint boundary condition to obtain non-collocated sensitivities is also discussed. Second, we present results that demonstrate the application of the theory to a two-dimensional inverse design problem using the traditional Ni-bump geometry.

Keywords: Discrete Adjoint; Optimization; Non-Collocated Sensitivities; Euler; Ni-Bump; Supersonic

1. Introduction

The mathematical theory for control systems governed by partial differential equations has created a framework for the formulation of inverse design and general aerodynamic problems at a reduced computational cost, as shown by Bauer et al. [1], Garabedian et al. [2], Hicks et al. [3], Lions et al. [4], and Pironneau et al. [5]. Recently, with the help of faster computing resources, automatic aerodynamic optimization has been revisited by Jameson et al. [6, 7, 8, 9, 10]. Optimization techniques for the design of aerospace vehicles generally use gradient-based methods and traditionally, finite difference methods have been used to calculate the sensitivity derivatives of the aerodynamic cost function. The computational

cost of the finite difference method for problems involving large numbers of design variables is unaffordable. The mathematical theory for the control of systems governed by partial differential equations, as developed by Lions et al. [4], significantly lowers the computational cost and is clearly an improvement over classical finite-difference methods.

Using control theory the gradient is calculated indirectly by solving an adjoint equation. Although there is the additional overhead of solving the adjoint equation, once it has been solved the cost of obtaining the sensitivity derivatives of the cost function with respect to each design variable is negligible. Consequently, the total cost to obtain these gradients is independent of the number of design variables and amounts to the cost of one flow solution and one adjoint solution. The adjoint problem is a linear PDE of lower complexity than the flow solver. This method was first applied to transonic flow by Jameson et al. [6]. In the last six years automatic aerodynamic design of complete aircraft configurations has yielded optimized solutions of wing and wing-body configurations by Reuther et al. [11, 12] and Burgreen et al. [13].

The adjoint equation can be derived using either a continuous or discrete approach. The discrete adjoint approach applies control theory directly to the discrete field equations. The discrete adjoint equation is then derived by collecting together all the terms multiplied by the variation $\delta w_{i,j}$ of the discrete flow variables. A detailed comparison of the continuous and discrete adjoint approaches was conducted by Nadarajah et al. [14]. Extensive work on the discrete adjoint method has also been contributed by Shubin et al. [15], Beux et al. [16], Elliot et al. [17], Anderson et al. [18], Iollo et al. [19], and Ta'saan et al. [20]

Traditional adjoint implementations were aimed at reducing a cost function computed from the pressure distribution on the surface that is being modified. In this case, however, we would like to obtain sensitivity derivatives of pressure distributions that are not collocated at the points where the geometry is being modified. This type of sensitivity calculation has not been attempted before and will be necessary for a variety of problems including sonic boom minimization, inlet design, turbomachinery design, etc.

2. Design Using the Euler Equations

For the flow in a nozzle, the aerodynamic properties that define the cost function are assumed to be functions of both the flow-field variables, w, and the physical location of the boundary. Using control theory, the governing equations of the flow-field can be introduced as a constraint in such a way that the final expression for the gradient does not require reevaluation of the flow-field.

The discrete adjoint equation is obtained by applying control theory directly to the set of discrete field equations. The resulting equation depends on the type of scheme used to discretize the flow equations. The work in this paper uses a cell centered multigrid scheme with upwind-biased blended first-and-third-order fluxes for artificial dissipation, local time stepping, and implicit residual smoothing. A full discretization of the equation would involve discretizing every term that is a function of the state vector. The variation of the cost function, δI, can be augmented by the discrete governing equations appropriately premultiplied by the adjoint variable $\psi_{i,j}^T$.

$$\delta I = \frac{1}{2} \sum_{B_{UpperWall}} (p - p_d)^2 \ \Delta s + \sum_{i=2}^{nx} \sum_{j=2}^{ny} \psi_{i,j}^T \delta \left(R\left(w\right)_{i,j} + D\left(w\right)_{i,j} \right), \tag{1}$$

where the first term represents the discrete cost function, $R(w)$ is the field equation, and $D(w)$ is the artificial dissipation term.

In order to eliminate δw from Eq (1), terms multiplied by the variation $\delta w_{i,j}$ of the discrete flow variables are collected and equated to zero. The following is the resulting discrete adjoint equation,

$$\begin{aligned} V \frac{\partial \psi_{i,j}}{\partial t} = & \left(\Delta y_{\eta_{i+\frac{1}{2},j}} \left[\frac{\partial f}{\partial w} \right]_{i,j}^T - \Delta x_{\eta_{i+\frac{1}{2},j}} \left[\frac{\partial g}{\partial w} \right]_{i,j}^T \right) \left(\frac{\psi_{i+1,j}}{2} - \frac{\psi_{i,j}}{2} \right) + \delta d_{i+\frac{1}{2},j} \\ & + \left(\Delta y_{\eta_{i-\frac{1}{2},j}} \left[\frac{\partial f}{\partial w} \right]_{i,j}^T - \Delta x_{\eta_{i-\frac{1}{2},j}} \left[\frac{\partial g}{\partial w} \right]_{i,j}^T \right) \left(\frac{\psi_{i,j}}{2} - \frac{\psi_{i-1,j}}{2} \right) - \delta d_{i-\frac{1}{2},j} \\ & + \left(\Delta x_{\xi_{i,j+\frac{1}{2}}} \left[\frac{\partial g}{\partial w} \right]_{i,j}^T - \Delta y_{\xi_{i,j+\frac{1}{2}}} \left[\frac{\partial f}{\partial w} \right]_{i,j}^T \right) \left(\frac{\psi_{i,j+1}}{2} - \frac{\psi_{i,j}}{2} \right) + \delta d_{i,j+\frac{1}{2}} \\ & + \left(\Delta x_{\xi_{i,j-\frac{1}{2}}} \left[\frac{\partial g}{\partial w} \right]_{i,j}^T - \Delta y_{\xi_{i,j-\frac{1}{2}}} \left[\frac{\partial f}{\partial w} \right]_{i,j}^T \right) \left(\frac{\psi_{i,j}}{2} - \frac{\psi_{i,j-1}}{2} \right) - \delta d_{i,j-\frac{1}{2}}, \end{aligned} \tag{2}$$

where,

$$\delta d_{i+\frac{1}{2},j} = \epsilon^2_{i+\frac{1}{2},j}(\psi_{i+1,j} - \psi_{i,j}) - \epsilon^4_{i+\frac{3}{2},j}\psi_{i+2,j} + 3\epsilon^4_{i+\frac{1}{2},j}\left(\psi_{i+1,j} - \psi_{i,j}\right) + \epsilon^4_{i-\frac{3}{2},j}\psi_{i-1,j}, \tag{3}$$

is the discrete adjoint artificial dissipation term and V is the cell area. The dissipation coefficients ϵ^2 and ϵ^4 are functions of the flow variables, but, in order to reduce complexity, they are treated as constants. The effect of this partial discretization has been explored by Nadarajah et al. [14].

2.1 Discrete Adjoint Boundary Condition

This section illustrates the development of the discrete adjoint boundary condition for the calculation of non-collocated sensitivities for supersonic flow in a Ni-bump nozzle. The $\delta w_{i,UW}$ (where UW denotes the cells along the upper wall) term from the discrete cost function is added to the corresponding term from Eq (2). The discrete boundary condition appears as a source term in the adjoint fluxes. For example, at cell (i, UW) the adjoint equation can be discretized as follows,

$$\begin{aligned} V\frac{\partial \psi_{i,UW}}{\partial t} &= \frac{1}{2}\left[-A^T_{i-\frac{1}{2},UW}\left(\psi_{i,UW} - \psi_{i-1,UW}\right) - A^T_{i+\frac{1}{2},UW}\left(\psi_{i+1,UW} - \psi_{i,UW}\right)\right] \\ &\quad + \frac{1}{2}\left[-B^T_{i,\frac{5}{2}}\left(\psi_{i,3} - \psi_{i,UW}\right)\right] + \Phi, \end{aligned} \tag{4}$$

where V is the cell area, Φ is the source term for inverse design,

$$\Phi = \left(-\Delta y_\xi \psi_{2_{i,UW}} + \Delta x_\xi \psi_{3_{i,UW}} - (p - p_T)\Delta s_i\right)\delta p_{i,UW},$$

and

$$A^T_{i+\frac{1}{2},UW} = \Delta y_{\eta_{i+\frac{1}{2},UW}}\left[\frac{\partial f}{\partial w}\right]^T_{i,UW} - \Delta x_{\eta_{i+\frac{1}{2},UW}}\left[\frac{\partial g}{\partial w}\right]^T_{i,UW}.$$

If a first order dissipation scheme is used, then Eq (3) would reduce to the term associated with ϵ^2. In such a case, the discrete adjoint equations are completely independent of the costate variables in the cells below the wall. However, if we use the blended first-and-third-order scheme, these flow variable values are required. A simple zeroth-order extrapolation

across the wall has produced good results, as shown by Nadarajah et al. [14]. At cell (i, LW) (where LW denotes the cells along the lower wall), the adjoint fluxes and boundary conditions are similar to Eq (4), except that the source term does not contributions from the discrete cost function.

2.2 Optimization Procedure

In this paper, the inverse design boundary condition is applied to the upper wall while sensitivity derivatives or the gradient are calculated along the lower wall. The gradient for the discrete adjoint is obtained by perturbing each point on the lower wall. Once the gradient $\mathcal{G} = \frac{\partial I}{\partial b}$ has been determined, it can be used to drive a variety of gradient-based search procedures. The search procedure used in this work is a simple descent method in which small steps are taken in the negative gradient direction. Let $\mathcal{F}$ represent the design variable, and $\mathcal{G}$ the gradient. Then an improvement can be made with a shape change

$$\delta\mathcal{F} = -\lambda\mathcal{G}.$$

The gradient $\mathcal{G}$ can be replaced by a smoothed value $\bar{\mathcal{G}}$ in the descent process. This acts as a preconditioner which allows the use of much larger steps and ensures that each new shape in the optimization sequence remains smooth. To apply smoothing in the ξ_1 direction, the smoothed gradient $\bar{\mathcal{G}}$ may be calculated from a discrete approximation to

$$\bar{\mathcal{G}} - \frac{\partial}{\partial\xi_1}\epsilon\frac{\partial\bar{\mathcal{G}}}{\partial\xi_1} = \mathcal{G}, \;\; \bar{\mathcal{G}} = 0 \quad \text{at end points,}$$

where ϵ is the smoothing parameter. If the modification is applied on the surface $\xi_2 =$ constant, then the first order change in the cost function is

$$\begin{aligned}
\delta I &= -\int\int \mathcal{G}\delta\mathcal{F} d\xi_1 \\
&= -\lambda\int\int\left(\overline{\mathcal{G}} - \frac{\partial}{\partial\xi_1}\epsilon\frac{\partial}{\partial\xi_1}\overline{\mathcal{G}}\right)\overline{\mathcal{G}} d\xi_1 \\
&= -\lambda\int\int\left(\overline{\mathcal{G}}^2 + \epsilon\left(\frac{\partial\overline{\mathcal{G}}}{\partial\xi_1}\right)^2\right) d\xi_1 \\
&< 0,
\end{aligned}$$

again guaranteeing an improvement unless $\bar{\mathcal{G}} = \mathcal{G} = 0$ and assuring an improvement if λ is sufficiently small and positive.

This proves to be an extremely effective preconditioner. In some problems it turns out that the Hessian can be represented as a second order differential operator, so that with a proper choice of the smoothing parameter, the method becomes the Newton method. Search methods were intensively evaluated in a recent study by Jameson et al. [21], and it was verified that these sample problems (which may have a high linear content) could be solved with a number of search steps independent of the number of design variables.

2.3 Results

In order to validate the use of this new method for the calculation of flow sensitivities, we have constructed the following test problem, based on the Ni-bump geometry with a longer downstream portion of the channel. A channel of unit height and length, $l = 8.0$ is constructed. A 1.8% thick Ni-bump of unit chord is centered about $x = 6.0$. Along the upper wall, a target pressure corresponding to the presence of the same Ni-bump centered about $x = 2.0$ is specified, and the geometry of the complete lower surface of the channel is allowed to move so that the target pressure is obtained. Clearly, the solution of this problem is the disappearance of the initial bump, and the formation of the exact same bump centered about $x = 2.0$.

Figure 1 illustrates the non-dimensional pressure contours of a typical Euler solution on the final configuration. Figure 2 shows the initial and final (red and blue respectively) geometries of the lower wall as explained above. Notice that the aspect ratio of the figure on the right has been modified so that the small thickness Ni-bumps are visible. A more interesting set of plots are those of the pressure distributions on the upper surface of the channel before and after the optimization process has been completed. Figure 3 illustrates the initial pressure distribution corresponding to the Ni-bump centered about $x = 6.0$ (in red), while the target pressure distribution along the upper surface of the bump is in blue. After

60 design iterations, using the adjoint procedure described above for the computation of the sensitivities, Figure 4 illustrates that the target pressure distribution along the upper surface is very closely matched. The Ni-bump centered about $x = 6.0$ has completely disappeared, while its twin centered about $x = 2.0$ has formed.

3. Conclusions

This paper presents a complete formulation for the adjoint-based calculation of non-collocated sensitivities in supersonic flow. Boundary conditions and source terms for inverse design problems using a discrete adjoint approach were developed. Furthermore the feasibility of this method has been validated in the design of Ni-bumps on the lower wall of a nozzle created to achieve a target pressure distribution on the upper wall. Knowledge acquired through this effort will be applied to sonic boom minimization and turbomachinery problems.

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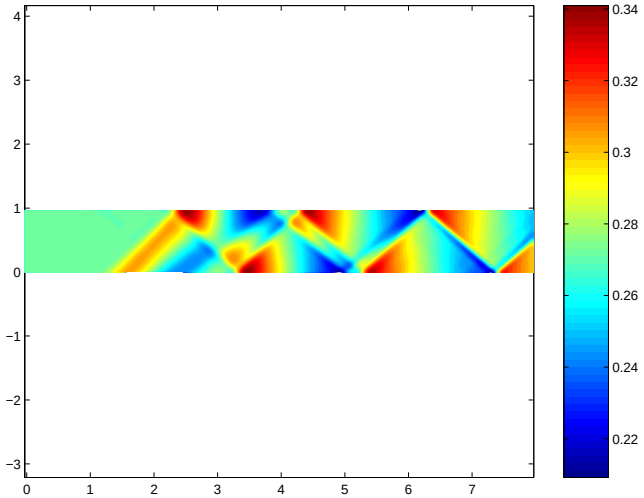

Figure 1: Final Solution Pressure Contours for Ni-Bump Geometry

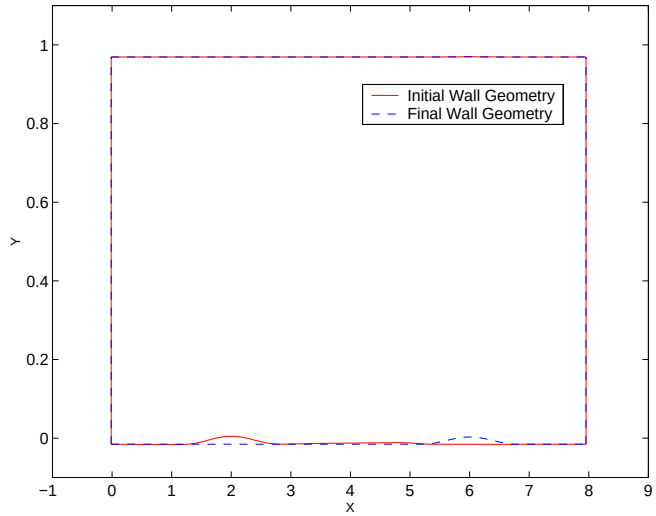

Figure 2: Initial and Final Lower Ni-bump Wall Geometry

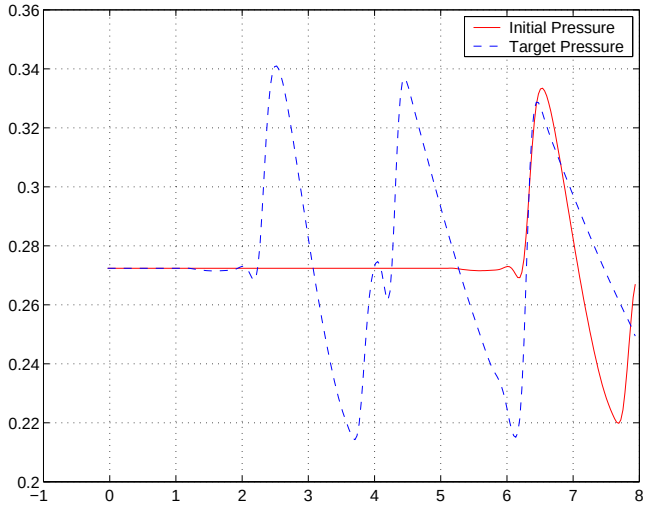

Figure 3: Initial Upper Surface Pressure Distributions.

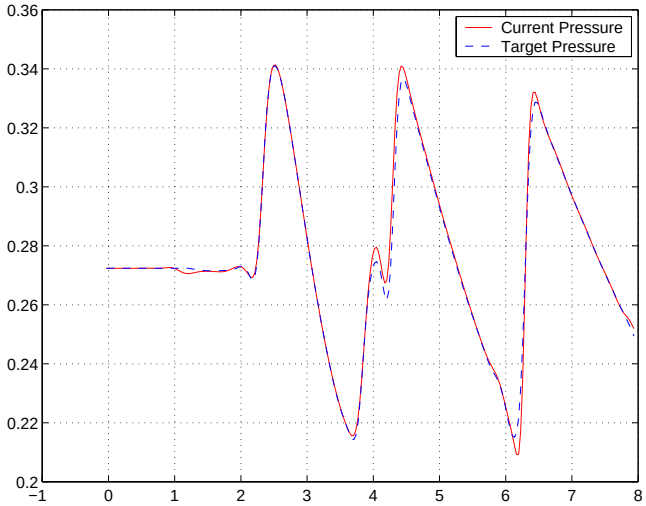

Figure 4: Final Upper Surface Pressure Distributions.