APPENDIX D

NUMERICALLY EXACT JACOBIAN ESTIMATION

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The Jacobian matrix of the vector of equations $W(Q) = 0$ resulting from the discretized system of differential equations, or an approximation of the Jacobian, is needed for implicit solution of the system of equations. Depending on the nature of the flow solver solution algorithm, inexact Jacobians can be employed. These inexact Jacobians may represent the Jacobian for a lower order discretization of the differential equations, or they may neglect or simplify complicated terms, such as those resulting from turbulence models, upwinding schemes and flux limiters. Because of these simplifications, the inexact Jacobians are easier to code and are more computationally efficient to calculate. In the case of lower order Jacobians, the resulting system of equations is also easier to solver. As a result, many implicit codes rely on inexact Jacobians. Within discrete sensitivity analysis, the errors in the inexact Jacobian affect the accuracy of the design space derivatives. Thus, to obtain the most accurate derivatives, the Jacobian matrix must be numerically exact.

Three alternatives are available for the calculation of numerically exact Jacobians - automatic differentiation, finite differences and a complex arithmetic approach. Automatic differentiation offers analytically exact derivatives by introducing the derivatives of each relevant equation into the code. In ADIFOR, the user would tell the code to determine the derivatives of the discretized equations W with respect to the flow variables Q, in order to calculate the Jacobian matrix. But since the Jacobian matrix is quite sparse, this approach would result in the calculation of the entire matrix and thereby incurring an unreasonably large computational expense. By using ADIFOR in a more creative way, a user may be able to calculate the Jacobian matrix in a much more efficient fashion, as in the paper by Corliss, etal **[70]**.

To calculate the entry $\frac{\partial W_i}{\partial Q_j}$ in the Jacobian via finite differences, the central difference formula can be used

$$\frac{\partial W_i(\vec{Q})}{\partial Q_j} \approx \frac{W_i(\vec{Q} + e_j \Delta Q) - W_i(\vec{Q} - e_j \Delta Q)}{2\Delta Q} \tag{D.1}$$

The drawback of this technique is that subtraction error limits the accuracy of the derivatives. Nevertheless, this method has been used in many implicit codes.

Finally, the entries in the Jacobian can be calculated via the complex Taylor's series expansion (CTSE) method by observing the Taylor's series expansion of

$$W_i(\vec{Q} + ie_j \Delta Q) = W_i(\vec{Q}) + i\frac{\partial W_i}{\partial Q_j}\Delta Q - \frac{\partial^2 W_i}{\partial^2 Q_j}(\Delta Q)^2 - i\frac{\partial^3 W_i}{\partial^3 Q_j}(\Delta Q)^3 + O((\Delta Q)^4) \tag{D.2}$$

where $i = \sqrt{-1}$. By considering the imaginary part of the equation, one can solve for the first derivative term,

$$Im(W(\vec{Q} + ie_j \Delta Q)) = \frac{\partial W_i(\vec{Q})}{\partial Q_j}\Delta Q + O((\Delta Q)^3) \tag{D.3}$$

or

$$\frac{\partial W_i(\vec{Q})}{\partial Q_j} = \frac{Im(W(\vec{Q} + ie_j \Delta Q))}{\Delta Q} + O((\Delta Q)^2) \tag{D.4}$$

By choosing ΔQ such that $O((\Delta Q)^2)$ terms are less than machine precision, the derivative can be approximated to within machine accuracy, without any subtraction error. The disadvantage of this technique over finite differences is that complex arithmetic is more computationally expensive. Therefore, this technique should be used to estimate the Jacobian matrix only when a highly accurate Jacobian matrix is needed. The complex Taylor's series expansion method is used to generate the numerically exact Jacobians within the discrete sensitivity analysis subroutines in this research. Whitfield and Taylor [**21**] also used the CTSE method to generate numerically exact Jacobians.

In addition to generating exact Jacobians for implicit codes, the complex Taylor's series expansion method can be used to generate exact Jacobians for explicit codes. At steady-state, an implicit code and an explicit code solve the same equation. Thus, the Jacobian matrix is the same. Using this method, the discrete form of sensitivity analysis can be applied to explicit codes, which was not possible without the costly expense of hand-differentiating the explicit formulas to obtain the analytic Jacobian.