Appendices

A. Sensitivity of the Van Leer Fluxes

The flux Jacobians of the inviscid flux vector in Eq.(3.2), and the Van Leer fluxes in Eq.(3.11), can be found in the literature [9,172,173] and are therefore omitted here. The sensitivity of the Van Leer fluxes, for higher-order spatially accurate discrete sensitivity analysis on unstructured grids, has been performed and presented for the first time in the current research. These sensitivities may be derived by noting that for unstructured grids there are two means by which the mesh dependence on the design variables may influence the flux vector; the metric terms, $N = \begin{cases} x & y \\ y & z \end{cases}^T$, the cell face area, A_f , and the upwind interpolation scheme, $Q_f = \{ u \ v \ w \ p\}^T$. These dependencies may be symbolically written for the residual vector as

$$\frac{R}{X} \frac{X}{k} = \lim_{j=(i)} \frac{E_{i,j}^{+}}{N} \frac{N}{k} + \frac{E_{i,j}^{-}}{N} \frac{N}{k} + \frac{E_{i,j}^{-}}{Q_{f}^{-}} \frac{Q_{f}^{-}}{k} + \frac{E_{i,j}^{-}}{Q_{f}^{+}} \frac{Q_{f}^{+}}{k} A_{i,j} + \left(E_{i,j}^{+} + E_{i,j}^{-}\right) \frac{A_{i,j}}{k}$$
(A.1)

Recall from section 3.1.2, that the determination of the appropriate fluxes are based upon the Mach number normal to the cell face. For supersonic flow through the cell face, the flux vector given by Eq.(3.2) is used with the primitive variables interpolated to the cell interfaces. The sensitivity of this flux vector with respect to the metric dependence on the

design variables, i.e., $\frac{N}{k} = \frac{x}{k} \frac{y}{k} \frac{z}{k}$, may be expressed as

$$\frac{-\frac{1}{k}|_{Q_{f}}}{u-\frac{1}{k}|_{Q_{f}}} + p - \frac{x}{k}}$$

$$\frac{E}{N} \frac{N}{k} = v - \frac{1}{k}|_{Q_{f}}}{u-\frac{1}{k}|_{Q_{f}}} + p - \frac{y}{k}$$

$$W - \frac{1}{k}|_{Q_{f}}}{u-\frac{1}{k}|_{Q_{f}}}$$
(A.2a)

and with respect to the dependence of the upwind interpolation on the design variables

$$\frac{Q_f}{k} = \frac{u}{k} \frac{v}{k} \frac{w}{k} \frac{p}{k}^T \text{ as}$$

$$\frac{-\frac{w}{k} + \frac{w}{k}}{k} \frac{p}{k}^T \text{ as}$$

$$\frac{-\frac{w}{k} + \frac{w}{k}}{k} \frac{w}{k} \frac{w}{k} \frac{p}{k} \frac{p}{k} x \frac{w}{k} \frac$$

where the sensitivity of the normal velocity is the combination

$$\frac{1}{k} = \frac{1}{k} \left|_{Q_f} + \frac{1}{k} \right|_N \tag{A.3a}$$

with

$$\frac{1}{k} \Big|_{Q_f} = u \frac{x}{k} + v \frac{y}{k} + w \frac{z}{k}; \quad \frac{1}{k} \Big|_N = \frac{u}{k} \frac{x}{k} + \frac{v}{k} \frac{y}{k} + \frac{w}{k} \frac{z}{k}$$
(A.3b)

and the sensitivity of the total enthalpy is given by

$$\frac{\left(e_{o}+p\right)}{k} = \frac{p}{-1} \frac{p}{k} + \frac{u^{2}+v^{2}+w^{2}}{2} + \frac{u}{k} \frac{u}{k} + v \frac{v}{k} + w \frac{w}{k}$$
(A.4)

For subsonic flow through the cell face, the split Van Leer fluxes in Eq.(3.11) are utilized. The sensitivity of these fluxes may be expressed as

$$\frac{\underline{f_{mass}^{\pm}}}{k} = \frac{f_{mass}^{\pm} f_{mom1}^{\pm} + f_{mass}^{\pm} \frac{f_{mom1}^{\pm}}{k}}{k} + \frac{E^{\pm}}{Q_{f}} \frac{Q_{f}}{k} = \frac{f_{mass}^{\pm} f_{mom2}^{\pm} + f_{mass}^{\pm} \frac{f_{mom2}^{\pm}}{k}}{k} + f_{mass}^{\pm} \frac{f_{mom3}^{\pm}}{k}}{k} + \frac{f_{mass}^{\pm} f_{mom3}^{\pm}}{k}} + f_{mass}^{\pm} \frac{f_{mom3}^{\pm}}{k}}{k}$$
(A.5)

where the sensitivity of the mass flux contains the contributions

$$\frac{f_{mass}^{\pm}}{k} = \frac{f_{mass}^{\pm}}{k} \bigg|_{Q_f} + \frac{f_{mass}^{\pm}}{k} \bigg|_{N}$$
(A.6a)

with

$$\frac{f_{mass}^{\pm}}{k}\Big|_{Q_f} = \pm \frac{a}{2} \left(M_n \pm 1 \right) \frac{M_n}{k} \Big|_{Q_f}$$
(A.6b)

$$\frac{f_{mass}^{\pm}}{k}\Big|_{N} = \pm \frac{1}{4} - \frac{1}{k} a(M_{n} \pm 1)^{2} + \frac{a}{k} (M_{n} \pm 1)^{2} + 2 a(M_{n} \pm 1) \frac{M_{n}}{k}\Big|_{N}$$
(A.6c)

The sensitivity of the f_{mom1}^{\pm} term is the combination

$$\frac{f_{mom1}^{\pm}}{k} = \frac{f_{mom1}^{\pm}}{k} \bigg|_{Q_f} + \frac{f_{mom1}^{\pm}}{k} \bigg|_{N}$$
(A.7a)

where

$$\frac{f_{mom1}^{\pm}}{k}\Big|_{Q_f} = \frac{x}{k} \left(-\pm 2a\right) / \left(-\frac{x}{k}\right) - \frac{x}{k}\Big|_{Q_f}$$
(A.7b)

$$\frac{f_{mom1}^{\pm}}{k}\bigg|_{N} = \frac{u}{k} + \frac{x}{k} - \frac{1}{k}\bigg|_{N} \pm 2\frac{a}{k}$$
(A.7c)

Analogous relations may be written for f_{mom2}^{\pm}/k and f_{mom3}^{\pm}/k . Similarly the sensitivity for the energy term is

$$\frac{f_e^{\pm}}{k} = \frac{f_e^{\pm}}{k} \bigg|_{Q_f} + \frac{f_e^{\pm}}{k} \bigg|_N$$
(A.8a)

where

$$\frac{f_e^{\pm}}{k}\Big|_{Q_f} = \frac{2}{2-1} \left[(1-1) \pm (-1)a \right] \frac{1}{k} \Big|_{Q_f}$$
(A.8b)

$$\frac{f_e^{\pm}}{k}\Big|_N = \frac{2}{2} \left\{ (1 - 1) \pm (1 - 1)a \right\} - \frac{1}{k} \Big|_N + \left\{ 2a \pm (1 - 1) \right\} - \frac{a}{k} + u \frac{u}{k} + v \frac{v}{k} + w \frac{w}{k}$$
(A.8c)

In the above equations the sensitivities of the normal Mach number are given by

$$\frac{M_n}{k}\Big|_{Q_f} = \frac{1}{a} \frac{1}{k}\Big|_{Q_f}; \quad \frac{M_n}{k}\Big|_N = \frac{1}{a} \frac{1}{k}\Big|_N - \frac{1}{a^2} \frac{a}{k}$$
(A.9)

where the sensitivity for the speed of sound is

$$\frac{a}{k} = \frac{1}{2a} \frac{1}{k} - \frac{p}{2} \frac{p}{k}$$
(A.10)

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As seen, the sensitivity of the inviscid split fluxes requires the determination of the sensitivity of the metric terms and the sensitivity of the upwind interpolation scheme. The evaluation of the metric terms on unstructured grids and the corresponding sensitivity of these terms are presented below in Appendix C. The sensitivity of the upwind interpolation scheme, using both the inverse-distance and the psuedo-Laplacian weighting methods, are presented in Appendix D.

B. Jacobians/Sensitivity of the Boundary Conditions

The boundary-condition types utilized in the current work are inviscid solid boundary (flow tangency) and characteristic inflow/outflow. These boundary conditions are those most commonly used in inviscid CFD analysis and may be easily found in the literature; for example, see reference 128. Furthermore, a first-order implementation of these boundary conditions is utilized in the current research. This implementation simply uses the cell center values of the primitive variables adjacent to the boundary faces as opposed to the interpolation of these variables to the boundary faces. A more detailed description and comparison of both implementations has been reported Ref. 129 for unstructured grid schemes. The most common approach, however, is the first-order one.

The boundary values of the primitive variables Q_b for flow tangency are specified as

$$b = o$$

$$u_{b} = u_{o} - o_{x}; \quad v_{b} = v_{o} - o_{y}; \quad w_{b} = w_{o} - o_{z}$$

$$p_{b} = p_{o}$$
(B.1)

where the normal velocity at the boundary is computed from the interior velocity components as

$$_{o} = u_{o x} + v_{o y} + w_{o z}$$
 (B.2)

The state equation for the boundary conditions may be express as

$$B(Q_{o},Q_{b},X) = \begin{array}{c} v_{o} - v_{b} \\ v_{o} - v_{o} - v_{b} \\ w_{o} - v_{c} - v_{b} \\ p_{o} - p_{b} \end{array} = 0$$
(B.3)

The Jacobian of this state equation, with respect to the interior state variables, is derived as

and with respect to the state variables on the boundary

$$\frac{B}{Q_b} = -\left[\overline{\overline{I}}\right] = \frac{B}{Q_b}^{-1}$$
(B.5)

where \overline{I} is the identity matrix. The inverse of this matrix is required in the sensitivity analysis using either the pre-eliminated form of the sensitivity equation (e.g., Eqs.(3.26a and b)) or the incremental form (e.g., Eq.(4.12)).

The sensitivity of the boundary state equation with respect to the design variables for the flow tangency condition may be written as

$$0$$

$$-\frac{o}{k}x + o\frac{x}{k}$$

$$\frac{B}{X}\frac{X}{k} = -\frac{o}{k}y + o\frac{y}{k}$$

$$-\frac{o}{k}z + o\frac{z}{k}$$
(B.6)

where

$$\frac{o}{k} = u_o \frac{x}{k} + v_o \frac{y}{k} + w_o \frac{z}{k}$$
(B.7)

For characteristic inflow/outflow boundary conditions, the Riemann invariants corresponding to the incoming and outgoing waves traveling in the characteristic directions defined normal to the boundary are applied at the far-field. The two locally one-dimensional Riemann invariants are given by

$$R^{+} = {}_{o} + \frac{2a_{o}}{-1}; \quad R^{-} = -\frac{2a}{-1}$$
 (B.8)

where $_{o}$ is given above and

$$a_o = \frac{p_o}{o}^{1/2}; a = \frac{p}{o}^{1/2}; = u_x + v_y + w_z$$
 (B.9)

The invariants are used to determine the locally normal velocity and speed of sound

$$- = \frac{1}{2} \left(R^+ + R^- \right); \quad \bar{a} = \frac{-1}{4} \left(R^+ - R^- \right)$$
(B.10)

For outflow (- > 0) on the boundary, the velocities are defined as

whereas for inflow (- < 0) on the boundary

$$u_b = u + x(-); v_b = v + y(-); w_b = w + z(-)$$
 (B.12)

The density on the boundary is computed from the entropy relation

$$b = \frac{\bar{a}^2}{S} \frac{1}{-1}$$
 (B.13)

with the entropy function S evaluated as

$$->0$$
 $S = S_o = \frac{p_o}{o};$ $-<0$ $S = S = \frac{p}{-1}$ (B.14)

Then the corresponding pressure on the boundary is computed from the equation of state

$$p_b = -\frac{b \bar{a}^2}{(B.15)}$$

Denoting for outflow *o* and for inflow , these boundary conditions may be written in state equation form as

$$B(Q_{o},Q_{b},X) = \begin{array}{c} \frac{\overline{a}^{2}}{S} & \frac{1}{-1} \\ u + x \left(- - \right) \\ v + y \left(- - \right) \\ w + z \left(- - \right) \\ - v_{b} \\ w + z \left(- - \right) \\ - w_{b} \\ - \frac{b\overline{a}^{2}}{-} - p_{b} \end{array}$$
(B.16)

The Jacobians of the state equation with respect to the interior state vector, for characteristic inflow/outflow boundary conditions may be derived as

$$\frac{1}{2} \frac{1}{1} \frac{1}{1} \frac{1}{u_0} \frac{1}{v_0} \frac{1}{v_0} \frac{1}{w_0} \frac{1}{u_0} \frac{1}{v_0} \frac{1}{v_0}$$

where

$$_{1} = \frac{2\bar{a}}{(-1)S} \frac{\bar{a}^{2}}{S}$$
(B.17b)

$$_{1} = \frac{\overline{a}}{o} - \frac{\overline{a}}{2S} \quad \frac{S}{o}; \qquad _{2} = \frac{\overline{a}}{p_{o}} - \frac{\overline{a}}{2S} \quad \frac{S}{p_{o}}$$
(B.17c)

and

$$_{3} = \frac{1}{u_{o}} - \frac{1}{u_{o}}; \quad _{4} = \frac{1}{v_{o}} - \frac{1}{v_{o}}; \quad _{5} = \frac{1}{w_{o}} - \frac{1}{w_{o}}$$
 (B.17d)

$$_2 = 2 \ _b \overline{a} / \tag{B.17e}$$

where = 1 for outflow (o) and = 0 for inflow (). The derivatives of the local normal velocity and speed of sound are

$$\frac{-}{Q_{o}} = \frac{-}{/} \frac{a}{u_{o}} = \frac{-\frac{p_{o}}{2(-1)a_{o}}^{2}}{-\frac{1}{u_{o}}}; \frac{\overline{a}}{\frac{x}{2}} = \frac{-1}{2} \frac{-}{Q_{o}}$$
(B.17f)
$$\frac{-}{/} \frac{w_{o}}{p_{o}} = \frac{-1}{2} \frac{-}{Q_{o}}$$

The derivative of the normal velocity for inflow () is zero, and for outflow

$$\frac{o}{Q_o} = \left\{ 0 \quad x \quad y \quad z \quad 0 \right\}^T \tag{B.17g}$$

For the state variables on the boundary

$$\frac{B}{Q_b} = -\left[\overline{\overline{I}}\right] + Elem(5,1); \qquad Elem(5,1) = \overline{a}^2/$$
(B.18)

Once again, the inverse of this matrix is needed in the sensitivity analysis, and from the above form, the inverse is simply

$$\frac{B}{Q_b}^{-1} = -\left[\bar{I}\right] - Elem(5,1)$$
(B.19)

That is, only a change in sign of the element in location (5,1) is required for the inverse.

The sensitivity of the boundary state equation with respect to the design variables is given by

$$\frac{2\bar{a}}{(-1)S} \frac{\bar{a}^{2}}{S} \frac{\bar{a}^{-1}}{\bar{a}} \frac{\bar{a}}{\bar{k}}$$

$$\frac{-\frac{x}{k}(\bar{a}-1)S}{\bar{b}} \frac{\bar{a}^{2}}{S} \frac{\bar{a}^{-1}}{\bar{b}} \frac{\bar{a}}{\bar{k}}$$

$$\frac{-\frac{x}{k}(\bar{a}-1)S}{\bar{b}} + \frac{\bar{b}^{-1}}{\bar{b}} \frac{\bar{b}^{-1}}{\bar{b}} \frac{\bar{b}^{-1}}{\bar{b}}$$

$$\frac{-\frac{x}{k}(\bar{a}-1)S}{\bar{b}} \frac{\bar{b}^{-1}}{\bar{b}} \frac{\bar{b}^{-1}}{\bar{b}}$$

with the local speed of sound and normal velocity sensitivity given by

$$\frac{\overline{a}}{k} = \frac{-1}{4} \left(u_o - u \right) \frac{x}{k} + \left(v_o - v \right) \frac{y}{k} + \left(w_o - w \right) \frac{z}{k}$$
(B.21)

$$\frac{-}{k} = \frac{1}{2} \left(u_o + u_b \right) - \frac{x}{k} + \left(v_o + v_b \right) - \frac{y}{k} + \left(w_o + w_b \right) - \frac{z}{k}$$
(B.22)

and where

$$\frac{1}{k} = \frac{1}{2} u \frac{x}{k} + v \frac{y}{k} + w \frac{z}{k}$$
(B.23)

is computed based on either an inflow or outflow condition.

The sensitivity of the boundary state equation, like the sensitivity of the flux vectors for the interior cell state equation discussed in Appendix A, require the metric sensitivity derivatives. The evaluation of the metric terms on an unstructured grid, and the corresponding sensitivity, are discussed in Appendix C.

C. Sensitivity of the Metric Terms

Expressions for the metric terms, and the corresponding sensitivity of these expressions, may be derived for a typical tetrahedral cell (see Fig. C.1) by first defining the edge vectors

$$L_{2} = \left\{ l_{2}^{x} \quad l_{2}^{y} \quad l_{2}^{z} \right\}^{T} = \left\{ \left(x_{n2} - x_{n1} \right) \quad \left(y_{n2} - y_{n1} \right) \quad \left(z_{n2} - z_{n1} \right) \right\}^{T}$$
(C.1a)

$$L_{3} = \left\{ l_{3}^{x} \quad l_{3}^{y} \quad l_{3}^{z} \right\}^{T} = \left\{ \left(x_{n3} - x_{n1} \right) \quad \left(y_{n3} - y_{n1} \right) \quad \left(z_{n3} - z_{n1} \right) \right\}^{T}$$
(C.1b)

$$L_{4} = \left\{ l_{4}^{x} \quad l_{4}^{y} \quad l_{4}^{z} \right\}^{T} = \left\{ \left(x_{n4} - x_{n1} \right) \quad \left(y_{n4} - y_{n1} \right) \quad \left(z_{n4} - z_{n1} \right) \right\}^{T}$$
(C.1c)

where the sensitivities of these vectors with respect to the shape design variables are

$$\frac{L_2}{k} = \frac{l_2^x}{k} \frac{l_2^y}{k} \frac{l_2^z}{k} \frac{l_2^z}{k}$$
(C.2a)

$$\frac{L_3}{k} = \frac{l_3^x}{k} \frac{l_3^y}{k} \frac{l_3^z}{k} \frac{l_3^z}{k}$$
(C.2b)

$$\frac{-L_4}{k} = \frac{-l_4^x}{k} - \frac{-l_4^y}{k} - \frac{-l_4^z}{k} - \frac{-l_4^z}{k}$$
(C.2c)

where, for example,

$$\frac{l_2^x}{k} = \frac{x_{n2}}{k} - \frac{x_{n1}}{k}; \quad \frac{l_2^y}{k} = \frac{y_{n2}}{k} - \frac{y_{n1}}{k}; \quad \frac{l_2^z}{k} = \frac{z_{n2}}{k} - \frac{z_{n1}}{k}$$
(C.3)

In Eq.(C.3) the quantities x_n/k , y_n/k , and z_n/k are the grid sensitivity terms discussed in Chapter 5. Similar expressions may be written for components of L_3/k and L_4/k . The area of face n1-n2-n3 may be computed as

$$A_{f} = \frac{1}{2} \left\| L_{2} \times L_{3} \right\| = \frac{1}{2} \left[a_{x}^{2} + a_{y}^{2} + a_{z}^{2} \right]^{\frac{1}{2}}$$

$$= \frac{1}{2} \left(l_{2}^{y} l_{3}^{z} - l_{2}^{z} l_{3}^{y} \right)^{2} + \left(l_{3}^{x} l_{2}^{z} - l_{2}^{x} l_{3}^{z} \right)^{2} + \left(l_{2}^{x} l_{3}^{y} - l_{3}^{x} l_{2}^{y} \right)^{2} \frac{1}{2}$$
(C.4)

with the sensitivity of the face area given by

$$\frac{A_f}{k} = \frac{A_f}{X} \frac{X}{k} = \frac{1}{4A_f} a_x \frac{a_x}{k} + a_y \frac{a_y}{k} + a_z \frac{a_z}{k}$$
(C.5)

where

$$\frac{a_x}{k} = \frac{l_2^y}{k} l_3^z + l_2^y \frac{l_3^z}{k} - \frac{l_2^z}{k} l_3^y + l_2^z \frac{l_3^y}{k}$$
(C.6a)

$$\frac{a_y}{k} = \frac{l_3^x}{k} l_2^z + l_3^x \frac{l_2^z}{k} - \frac{l_2^x}{k} l_3^z + l_2^x \frac{l_3^z}{k}$$
(C.6b)

$$\frac{a_z}{k} = \frac{l_2^x}{k} l_3^y + l_2^x \frac{l_3^y}{k} - \frac{l_3^x}{k} l_2^y + l_3^x \frac{l_2^y}{k}$$
(C.6c)

The normal direction, referred to as the direction cosines, for this face may be evaluated as

$$N = \left\{ \begin{array}{cc} x & y \\ x & z \end{array} \right\}^{T} = \frac{L_{2} \times L_{3}}{\|L_{2} \times L_{3}\|} = \frac{L_{2} \times L_{3}}{2A_{f}}$$
(C.7)

with the corresponding sensitivity

$$\frac{-N}{k} = \frac{N}{X} \frac{X}{k} = \frac{1}{2} - \frac{L_2}{k} \times L_3 + L_2 \times \frac{L_3}{k} - \frac{1}{A_f} - \frac{L_2 \times L_3}{(A_f)^2} \frac{A_f}{k}$$
(C.8)

Once again, similar expressions may be easily written for the other faces of the tetrahedron. The centroid of the tetrahedral cell is determined as

$$x_{c} = \frac{1}{4} \left(x_{n1} + x_{n2} + x_{n3} + x_{n4} \right)$$
(C.9a)

$$y_c = \frac{1}{4} \left(y_{n1} + y_{n2} + y_{n3} + y_{n4} \right)$$
(C.9b)

$$z_{c} = \frac{1}{4} \left(z_{n1} + z_{n2} + z_{n3} + z_{n4} \right)$$
(C.9c)

where

$$\frac{x_c}{k} = \frac{1}{4} \frac{x_{n1}}{k} + \frac{x_{n2}}{k} + \frac{x_{n3}}{k} + \frac{x_{n4}}{k}$$
(C.10a)

$$\frac{y_c}{k} = \frac{1}{4} \frac{y_{n1}}{k} + \frac{y_{n2}}{k} + \frac{y_{n3}}{k} + \frac{y_{n4}}{k}$$
(C.10b)

$$\frac{z_c}{k} = \frac{1}{4} \frac{z_{n1}}{k} + \frac{z_{n2}}{k} + \frac{z_{n3}}{k} + \frac{z_{n4}}{k}$$
(C.10c)

are the coordinate sensitivities of the centroid location.

D. Sensitivity of the Spatial Differencing

It was discussed in section 3.1.3, that the development of a higher-order spatially accurate scheme requires the interpolation of the state variables to the cell interfaces. For unstructured grid schemes, this interpolation is mesh dependent. Thus, the sensitivity of the interpolation given in Eq.(3.15) may be written as

$$\frac{Q_f^{\pm}}{k} = \frac{Q_f^{\pm}}{k} \begin{bmatrix} (Q + Q \quad \vec{r})^{\pm} \end{bmatrix} = \frac{Q_f^{\pm}}{k} \begin{bmatrix} (Q \quad \vec{r})^{\pm} \end{bmatrix}$$
(D.1a)

introducing the expression for the solution gradient in Eq.(3.16) yields

$$\frac{Q_f^{\pm}}{k} = \frac{1}{4} \frac{1}{3} \frac{Q_{n1}}{k} + \frac{Q_{n2}}{k} + \frac{Q_{n3}}{k} - \frac{Q_{n4}^{\pm}}{k}$$
(D.1b)

where the variables at the nodes are obtained from the multidimensional weighted averaging given in equation 3.17. The sensitivity of this averaging with respect to the design variables is given by

$$\frac{Q_n}{k} = \frac{nc}{i=1} \frac{w_{c,i}}{k} Q_{c,i} / \frac{nc}{i=1} w_{c,i} - \frac{nc}{i=1} w_{c,i} Q_{c,i} - \frac{nc}{i=1} \frac{w_{c,i}}{k} / \frac{nc}{i=1} \frac{2}{k}$$
(D.2)

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The sensitivity of the weighting factors, $w_{c,i}/k$, depends on the algorithm used. In the current research, an inverse-distance and a psuedo-Laplacian weighting procedure have been utilized. The sensitivity of each scheme is presented below.

D.1 Inverse Distance Weighting

The weighting factors for the inverse-distance procedure were given in equation 3.18. The sensitivity of these factors may be written as

$$\frac{w_{c,i}}{k} = -\frac{x \frac{(x)}{k} + y \frac{(y)}{k} + z \frac{(z)}{k}}{(x^2 + y^2 + z^2)^{3/2}}$$
(D.3)

with

$$\frac{(x)}{k} = \frac{x_{c,i}}{k} - \frac{x_n}{k}; \quad \frac{(y)}{k} = \frac{y_{c,i}}{k} - \frac{y_n}{k}; \quad \frac{(z)}{k} = \frac{z_{c,i}}{k} - \frac{z_n}{k}$$
(D.4)

where the sensitivity of the coordinates of the centroid location are given in equations C.10a through C.10c.

D.2 Psuedo-Laplacian Weighting

The weighting factors for this method have been given previously in equations 3.19a and 3.19b. Sensitivity of the weighting factors may be expressed as

$$\frac{w_{c,i}}{k} = \frac{x}{k} x + x \frac{(x)}{k} + \frac{y}{k} y + y \frac{(y)}{k} + \frac{z}{k} z + z \frac{(z)}{k}$$
(D.5)

where (x)/k, (y)/k, and (z)/k have been given above in equation D.4. The derivatives of the Lagrange multipliers may be expressed as

$$\frac{x}{k} = -\frac{1}{k} \left(\vec{I}^{y} \times \vec{I}^{z} \right) - \frac{\vec{I}^{y}}{k} \times \vec{I}^{z} + \vec{I}^{y} \times \frac{\vec{I}^{z}}{k}$$
(D.6a)

$$\frac{y}{k} = \frac{1}{k} \left(\vec{I}^x \times \vec{I}^z \right) + \frac{\vec{I}^x}{k} \times \vec{I}^z + \vec{I}^x \times \frac{\vec{I}^z}{k}$$
(D.6b)

$$\frac{z}{k} = -\frac{-}{k} \left(\overline{I}^x \times \overline{I}^y \right) - \frac{-}{k} \frac{\overline{I}^x}{k} \times \overline{I}^y + \overline{I}^x \times \frac{\overline{I}^y}{k}$$
(D.6c)

On examining the components of $\overline{}$, \overline{I}^x , \overline{I}^y , and \overline{I}^z , which are given in Eqs.(3.20d-i), it can be observed that the derivatives of these components only include the derivatives of the centroid location and nodal coordinates. Once again, the derivatives of the centroid location are given above in equations C.10a to C.10c.

E. Sensitivity of Common Output Functions

For aerodynamic calculations, typical output functions from which objective functions and constraints may be defined are the lift coefficient, drag coefficient, and lift-to-drag ratio. Each will be discussed to follow.

Lift Coefficient

The lift coefficient is computed as

$$C_L = \frac{F_z \cos - F_x \sin}{q A_{ref}}$$
(E.1)

where is the free-stream angle of attack, q is the dynamic pressure, A_{ref} is the reference area, and the forces in the *z*- and *x*-directions are

$$F_{z} = \prod_{j=1}^{nbf} {}_{z} A_{f}(p_{j} - p_{j}); \quad F_{x} = \prod_{j=1}^{nbf} {}_{x} A_{f}(p_{j} - p_{j})$$
(E.2)

where *nbf* is the number of boundary faces over which the pressure is integrated.

To compute the sensitivity derivatives in Eqs.(2.6a and b), the derivatives with respect to the state vector and the design variables are required. The derivatives of the lift coefficient are

$$\frac{C_L}{Q_i} = \begin{array}{c} 0\\ 0\\ 0\\ \frac{D_i}{Q_i} = \begin{array}{c} 0\\ nbf\\ ij A_f \left(z \cos - x \sin \right)\\ \frac{j=1}{q} A_{ref} \end{array}$$
(E.3)

where $_{ij}$ is the Kronecker delta, and

$$\frac{C_L}{X} \frac{X}{k} = \frac{nbf(p_j - p)}{j=1} \frac{1}{q} \frac{zA_f}{k} \cos -\frac{xA_f}{k} \sin$$
(E.4)

with

$$\frac{zA_f}{k} = \frac{A_{ref}}{A_{ref}} = \frac{A_{ref}}{k} = \frac{A_f}{k} + \frac{A_f}{k} - \frac{A_f}{k} + \frac{A_{ref}}{k}$$
(E.5)

A similar expression may be written for $\frac{xA_f}{A_{ref}}$. Note, if the reference area is fixed

throughout the design then the sensitivity of the reference area is zero. If the reference area used is the actual wetted surface area then the sensitivity of the reference area becomes

$$A_{ref} = \prod_{j=1}^{nbf} A_f; \qquad \frac{A_{ref}}{k} = \prod_{j=1}^{nbf} \frac{A_f}{k}$$
(E.6)

where the sensitivity of the face area has been given in Eq.(C.5) and the sensitivity of the metric terms are given in equation C.8.

Drag Coefficient

The drag coefficient is computed as

$$C_D = \frac{F_x \cos + F_z \sin}{q A_{ref}}$$
(E.7)

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with the derivatives of the drag coefficient given by

$$\frac{0}{0}$$

$$\frac{C_D}{Q_i} = \begin{array}{c} 0\\ nbf\\ ij A_f \left(x \cos + z \sin \right) \\ \underline{j=1} \\ q A_{ref} \end{array}$$
(E.8)

and

$$\frac{C_D}{X} \frac{X}{k} = \frac{nbf(p_j - p)}{j=1} \frac{xA_f}{q} \cos + \frac{zA_f}{A_{ref}} \sin$$
(E.9)

Note that the above assumes that the side slip angle is zero, but may be easily incorporated.

Lift-to-Drag Ratio

The derivatives of the lift-to-drag ratio may be expressed in terms of the derivatives of the lift coefficient and drag coefficient as follows

$$\frac{\left(C_L/C_D\right)}{Q} = \frac{C_L}{Q} - \frac{C_L}{C_D} \frac{C_D}{Q} / C_D$$
(E.10)

similarly

$$\frac{\left(C_{L}/C_{D}\right)}{X} \frac{X}{k} = \frac{C_{L}}{X} \frac{X}{k} - \frac{C_{L}}{C_{D}} \frac{C_{D}}{X} \frac{X}{k} / C_{D}$$
(E.11)

where all the terms in Eqs.(E.10 and E.11) have been given above.



Figure C.1: Typical unstructured grid tetrahedral cell.