APPENDIX B

THE MESH METRICS

In this section we will discuss the means by which the mesh metrics are derived and calculated. The expressions for F' and G' in equation (3.2.8) require the derivatives of the general coordinate system with respect to the Cartesian coordinates. However, we are unable to compute these derivatives, but we can calculate the derivatives of the Cartesian coordinates with respect to the general coordinates. With some algebra we can then relate the first to the second.

Equation (3.2.6) may be written as

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = \overbrace{\begin{pmatrix} \xi_x & \eta_x \\ \xi_y & \eta_y \end{pmatrix}}^{\mathbf{T}} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix}, \qquad (B.1)$$

where we have indicated a partial derivative as a subscript. We can write in a similar fashion

$$\begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix} = \underbrace{\begin{pmatrix} x_\xi & y_\xi \\ x_\eta & y_\eta \end{pmatrix}}_{\mathbf{T}^{-1}} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix}. \qquad (B.2)$$

If we use the fact that $\mathbf{T} = \left(\mathbf{T}^{-1}\right)^{-1}$, we have

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = \frac{1}{x_\xi y_\eta - y_\xi x_\eta} \begin{pmatrix} y_\eta & -y_\xi \\ -x_\eta & x_\xi \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix}, \qquad (B.3)$$

and thus equating like terms in equation (B.1), we have

$$
\begin{aligned}
\xi_x &= \frac{y_\eta}{x_\xi y_\eta - y_\xi x_\eta}, \qquad \eta_x = -\frac{y_\xi}{x_\xi y_\eta - y_\xi x_\eta}, \\
\xi_y &= -\frac{x_\eta}{x_\xi y_\eta - y_\xi x_\eta}, \qquad \eta_x = \frac{x_\xi}{x_\xi y_\eta - y_\xi x_\eta}.
\end{aligned} \tag{$B.4$}
$$

Thus knowing one set of metrics, we can compute the second set.

The derivatives of the Cartesian coordinates with respect to the general coordinate system are computed as follows. Note that, because we are using a finite volume mesh, the metrics are defined at the cell surfaces as indicated by the non-integer value of the indices.

$$
\begin{aligned}
\left.\frac{\partial x}{\partial \xi}\right|_{i,j+\frac{1}{2}} &= x_{i+1,j+1} - x_{i,j+1}, \qquad \left.\frac{\partial y}{\partial \xi}\right|_{i,j+\frac{1}{2}} = y_{i+1,j+1} - y_{i,j+1}, \\
\left.\frac{\partial x}{\partial \eta}\right|_{i+\frac{1}{2},j} &= x_{i+1,j+1} - x_{i+1,j}, \qquad \left.\frac{\partial y}{\partial \eta}\right|_{i+\frac{1}{2},j} = y_{i+1,j+1} - y_{i+1,j}.
\end{aligned} \tag{$B.4$}
$$

For convience, let us define the normalized metrics, which may also be thought of as the surface cosines to be

$$
\begin{aligned}
s'_{ix} &= \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}}, \qquad s'_{iy} = \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}}, \\
s'_{jx} &= \frac{\eta_x}{\sqrt{\eta_x^2 + \eta_y^2}}, \qquad s'_{jx} = \frac{\eta_y}{\sqrt{\eta_x^2 + \eta_y^2}}.
\end{aligned} \tag{$B.5$}
$$

These metrics will be useful in the discussion that follows in Appendix D.

APPENDIX C

THE FLUX JACOBIANS

The block matrices that are used to compute the split fluxes are presented here. The specific case of a gas composed of seven chemical species, four of which are diatomic and one is electrons, is presented here. The chemical species are ordered so that the diatomic species come first, then the monatomic species, and finally the electrons. The matrices are arranged in the same order as the flux vectors that are presented in equation (3.3.1) for example. Namely the first seven rows correspond to the density equations, the next two to the x and y momentum equations, the next four to the vibrational energy equations, and the last two to the electron and total energy equations.

The Jacobian $S = \frac{\partial V}{\partial U}$ that appears in equations (3.3.8) and (3.3.9) is shown on a following page, where the vector of non-conserved quantities, V, is given by equation (3.3.6). The partial derivatives of the pressure with respect to the conserved variables may be derived by writing p as a function of the conserved variables alone:

$$
\begin{aligned}
p = \frac{\sum_{s\neq e} \frac{\rho_s R}{M_s}}{\sum_{s\neq e} \rho_s c_{vs}} \Bigg[E - \sum_{s=1}^{4} E_{vs} - E_e - \frac{1}{2} \frac{\sum_{s\neq e} \rho_s}{\left(\sum_s \rho_s\right)^2} \left((\rho u)^2 + (\rho v)^2 \right) \\
- \sum_{s\neq e} \rho_s h_s^\circ - \sum_{s\neq e} \rho_s e_{\mathrm{el}s} \Bigg] \\
+ \frac{R}{M_e c_{ve}} \left[E_e - \frac{1}{2} \frac{\rho_e}{\left(\sum_s \rho_s\right)^2} \left((\rho u)^2 + (\rho v)^2 \right) \right].
\end{aligned}
\tag{C.1}
$$

Then differentiating this expression for p with respect to the conserved variables yields

$$
\begin{aligned}
\frac{\partial p}{\partial \rho_s} &= \Big(\frac{R}{M_s} - \frac{\bar{R} c_{vs}}{c_v}\Big) T + \frac{\bar{R}}{c_v}\big(\frac{1}{2}(u^2+v^2) - h_s^\circ - e_{\mathrm{els}}\big) \\
&\qquad\qquad\qquad + c_e\Big(\frac{R_e}{c_{ve}} - \frac{\bar{R}}{c_v}\Big)\big(u^2+v^2\big) \quad \text{for } s \neq e \\
\frac{\partial p}{\partial \rho_e} &= \Big(\frac{\bar{R}}{c_v} - \frac{1}{2}\frac{R_e}{c_{ve}}\Big)\big(u^2+v^2\big) + c_e\Big(\frac{R_e}{c_{ve}} - \frac{\bar{R}}{c_v}\Big)\big(u^2+v^2\big) \\
\frac{\partial p}{\partial \rho u} &= -u\left[\frac{\bar{R}}{c_v} + c_e\Big(\frac{R_e}{c_{ve}} - \frac{\bar{R}}{c_v}\Big)\right] \\
\frac{\partial p}{\partial \rho v} &= -v\left[\frac{\bar{R}}{c_v} + c_e\Big(\frac{R_e}{c_{ve}} - \frac{\bar{R}}{c_v}\Big)\right] \\
\frac{\partial p}{\partial E_{vs}} &= -\frac{\bar{R}}{c_v} \quad \text{for } s = 1, 4 \\
\frac{\partial p}{\partial E_e} &= \frac{R_e}{c_{ve}} - \frac{\bar{R}}{c_v} \\
\frac{\partial p}{\partial E} &= \frac{\bar{R}}{c_v}.
\end{aligned}
\tag{C.2}
$$

Where we have defined

$$
c_v = \sum_{s \neq e} \frac{\rho_s}{\rho} c_{vs}, \qquad \bar{R} = \sum_{s \neq e} \frac{\rho_s R}{\rho M_s}, \qquad R_e = \frac{R}{M_e}. \tag{C.3}
$$

In principle we could invert S to get S^{-1}, but it is easier to compute the Jacobian directly as $S^{-1} = \frac{\partial U}{\partial V}$. The expression obtained is given on a following page. The derivatives of E with respect to the non-conserved variables are computed by writing E in terms of these variables as

$$
\begin{aligned}
E = \frac{\sum_{s \neq e} \rho_s c_{vs}}{\sum_{s \neq e} \frac{\rho_s R}{M_s}} \left[p - \rho_e \frac{R_e}{c_{ve}}\big(e_e - \frac{1}{2}(u^2+v^2)\big)\right] + \sum_{s=1}^{4} \rho_s e_{vs} \\
+ \frac{1}{2}\sum_{s \neq e} \rho_s (u^2+v^2) + \sum_{s \neq e} \rho_s h_s^\circ + \sum_{s \neq e} \rho_s e_{\mathrm{els}}.
\end{aligned}
\tag{C.4}
$$

The derivatives that result are

$$
\begin{aligned}
\frac{\partial E}{\partial \rho_s} &= \Big(c_{vs} - \frac{c_v R}{M_s \bar{R}}\Big)T + e_{vs} + \frac{1}{2}(u^2+v^2) + h_s^\circ + e_{\mathrm{el}s} \quad \text{for } s = 1,4 \\
\frac{\partial E}{\partial \rho_s} &= \Big(c_{vs} - \frac{c_v R}{M_s \bar{R}}\Big)T + \frac{1}{2}(u^2+v^2) + h_s^\circ + e_{\mathrm{el}s} \quad \text{for } s = 5,6 \\
\frac{\partial E}{\partial \rho_e} &= e_e - \frac{c_v}{\bar{R}}\frac{R_e}{c_{ve}}\big(e_e - \frac{1}{2}(u^2+v^2)\big) \\
\frac{\partial E}{\partial u} &= \rho u\Big[1 - c_e\Big(1 - \frac{c_v}{\bar{R}}\frac{R_e}{c_{ve}}\Big)\Big] \\
\frac{\partial E}{\partial v} &= \rho v\Big[1 - c_e\Big(1 - \frac{c_v}{\bar{R}}\frac{R_e}{c_{ve}}\Big)\Big] \\
\frac{\partial E}{\partial e_{vs}} &= \rho_s \quad \text{for } s = 1,4 \\
\frac{\partial E}{\partial e_e} &= \rho_e\Big(1 - \frac{c_v}{\bar{R}}\frac{R_e}{c_{ve}}\Big) \\
\frac{\partial E}{\partial p} &= \frac{c_v}{\bar{R}}.
\end{aligned}
\tag{C.5}
$$

The Jacobian, $\frac{\partial V}{\partial U}\frac{\partial F_{\mathrm{I}}'}{\partial V}$, appearing in equation (3.3.5) is given below. It has been introduced because it is easier to diagonalize than the true Jacobian, $\frac{\partial F_{\mathrm{I}}'}{\partial U}$.

$$
\frac{\partial V}{\partial U}\frac{\partial F'}{\partial V} = \begin{pmatrix}
u' & 0 & \dots & 0 & \rho_1 & & & & \\
0 & u' & \dots & 0 & \rho_2 & & & & \\
\vdots & \vdots & \ddots & \vdots & \vdots & & & & \\
0 & 0 & \dots & u' & \rho_e & & & & \\
 & & & & u' & 0 & \dots & 0 & 1/\rho \\
 & & & & 0 & u' & \dots & 0 & 0 \\
 & & & & \vdots & \vdots & \ddots & \vdots & \vdots \\
 & & & & 0 & 0 & \dots & u' & 0 \\
 & & & & \rho a^2 & 0 & \dots & 0 & \tilde{u}'
\end{pmatrix}
\tag{C.6}
$$

The primes on the velocities indicate that they are velocities in the general coordinate directions. Thus u' is the velocity in the ξ direction and v' is in the η direction. They are defined in a fashion similar to the flux vectors F' and G', as in equation (3.2.8).

$$u' = \frac{\partial \xi}{\partial x} u + \frac{\partial \xi}{\partial y} v,$$
$$v' = \frac{\partial \eta}{\partial x} u + \frac{\partial \eta}{\partial y} v. \qquad (C.7)$$

The quantity $\tilde{u}'$ is a modified velocity due to the presence of electrons and is defined to be

$$\tilde{u}' = u' \Big(1 - c_e \Big(\frac{R_e}{c_{ve}} - \frac{\bar{R}}{c_v} \Big) \Big). \qquad (C.8)$$

The speed of sound, a, has been defined sush that

$$\rho a^2 = \sum_s \rho_s \frac{\partial p}{\partial \rho_s} + 2\rho u \frac{\partial p}{\partial \rho u} + \rho v \frac{\partial p}{\partial \rho v} + \sum_{s=1}^{4} E_{vs} \frac{\partial p}{\partial E_{vs}} + E_e \frac{\partial p}{\partial E_e} + \big[E + p + u \frac{\partial E}{\partial u} \big] \frac{\partial p}{\partial E}, \qquad (C.9)$$

which may be simplified using the derivatives given above to the expression

$$a^2 = \Big(1 + \frac{\bar{R}}{c_v} \Big) \big(\bar{R} T + c_e R_e T_e \big)$$
$$= \bar{\gamma} \big(\bar{R} T + c_e R_e T_e \big). \qquad (C.10)$$

Where we have defined $\bar{\gamma}$ to be the ratio of the frozen translational-rotational specific heats of the gas such that

$$\bar{\gamma} = 1 + \frac{\bar{R}}{c_v}. \qquad (C.11)$$

The above Jacobian, $\frac{\partial V}{\partial U} \frac{\partial F_{\mathrm{I}}'}{\partial V}$, is diagonalized with the characteristic matrix $C_{A'}$ as given in equation (3.3.7). Let us introduce the rotation matrix R_A, such that $C_{A'} = C_A \, R_A$, which has the effect of transforming the velocities between the general coordinates and the Cartesian coordinates. Then the Jacobian becomes

$$\frac{\partial V}{\partial U} \frac{\partial F_{\mathrm{I}}'}{\partial V} = R_A^{-1} \, C_A^{-1} \, \Lambda_{A'} \, C_A \, R_A, \qquad (C.12)$$

where R is the identity matrix except for rows 8 and 9

$$R_A = \begin{pmatrix} I & & & \\ & s'_{ix} & s'_{iy} & \\ & -s'_{iy} & s'_{ix} & \\ & & & I \end{pmatrix}. \tag{C.13}$$

The diagonal matrix of eigenvalues $\Lambda_{A'}$ represents the convection speeds of the characteristic variables and is given by

$$\Lambda_{A'} = \mathrm{diag}\left(\underbrace{u',\ u',\ \ldots,\ u'}_{7 \text{ elements}},\ \frac{1}{2}(u' + \tilde{u}') + \tilde{a},\ u',\ \underbrace{u',\ \ldots,\ u'}_{4 \text{ elements}},\ u',\ \frac{1}{2}(u' + \tilde{u}') - \tilde{a}\right)^T, \tag{C.14}$$

where $\tilde{a}$, a modified speed of sound, has been introduced such that

$$\tilde{a} = \sqrt{\left(\frac{u' - \tilde{u}'}{2}\right)^2 + a^2}. \tag{C.15}$$

Thus the presence of the electrons has an influence on the speed of sound, a, and on the effective speed of sound, $\tilde{a}$. The matrix C_A is determined by solving the eigenvalue problem and is given by

$$C_A = \begin{pmatrix} 1 & 0 & \ldots & 0 & \rho_1(\tilde{u}' - u')/a^2 & 0 & \ldots & 0 & -c_1/a^2 \\ 0 & 1 & \ldots & 0 & \rho_2(\tilde{u}' - u')/a^2 & 0 & \ldots & 0 & -c_2/a^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & \rho_e(\tilde{u}' - u')/a^2 & 0 & \ldots & 0 & -c_e/a^2 \\ & & & & \rho a^2/\tilde{a} & 0 & \ldots & 0 & a_+/\tilde{a} \\ & & & & 0 & 1 & \ldots & 0 & 0 \\ & & & & \vdots & \vdots & \ddots & \vdots & \vdots \\ & & & & 0 & 0 & \ldots & 1 & 0 \\ & & & & -\rho a^2/\tilde{a} & 0 & \ldots & 0 & a_-/\tilde{a} \end{pmatrix} \tag{C.16}$$

where the additional modified speeds of sound a_+ and a_- have been introduced for convenience. They are given by

$$
\begin{aligned}
a_+ &= \frac{1}{2}\big(\tilde{u}' - u'\big) + \tilde{a}, \\
a_- &= \frac{1}{2}\big(u' - \tilde{u}'\big) + \tilde{a}.
\end{aligned}
\tag{C.17}
$$

The inverse of C_A is a similarly sparse matrix

$$
C_A^{-1} = \begin{pmatrix}
1 & 0 & \dots & 0 & c_1/2a_+^2 & 0 & \dots & 0 & c_1/2a_-^2 \\
0 & 1 & \dots & 0 & c_2/2a_+^2 & 0 & \dots & 0 & c_2/2a_-^2 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
0 & 0 & \dots & 1 & c_e/2a_+^2 & 0 & \dots & 0 & c_e/2a_-^2 \\
 & & & & 1/2\rho a_+ & 0 & \dots & 0 & -1/2\rho a_- \\
 & & & & 0 & 1 & \dots & 0 & 0 \\
 & & & & \vdots & \vdots & \ddots & \vdots & \vdots \\
 & & & & 0 & 0 & \dots & 1 & 0 \\
 & & & & 1/2 & 0 & \dots & 0 & 1/2
\end{pmatrix}
\tag{C.18}
$$

The diagonalization procedure for the G', the flux vector in the η direction, is performed in the same fashion and yields analogous results.

The influence of the electrons on the speed of sound and the convection speeds is relatively minor. This can be seen by examining the order of magnitude of the ratio of $\tilde{u}'$ to u'. Consider the most severe case where the gas is composed of purely ions and electrons, then the molar concentration of each constituent is the same, and we have

$$
\frac{c_e}{M_e} = \frac{c_{\text{ions}}}{M_{\text{ions}}} \quad \text{and} \quad c_e + c_{\text{ions}} = 1. \tag{C.19}
$$

Solving these two equations yields that $c_e = O(10^{-5})$ for the molecular weight of NO^+, and thus the deviation of $\tilde{u}'$ from u' is at most of this order. Therefore the modified velocity, $\tilde{u}'$, could be replaced with u' and many of the matrices given above would simplify. Also all of the modified speeds of sound, $\tilde{a}$, a_+, and a_-, would revert to the speed of sound, a, defined in equation (C.9). However, the cost of keeping the additional terms is minimal, and in the computations that follow this was done.

APPENDIX D

THE IMPLICIT VISCOUS MATRICES

For the same case where we have seven chemical species, the general implicit viscous matrix M_η and the viscous matrix at the surface $i, 1\frac{1}{2}$ are given below. In the derivation of these matrices, we have assumed that the heat flux vector due to gradients of vibrational and electron temperature may be approximated in the following manner.

$$\begin{aligned} q_{vj} &= -\kappa_{vs}\frac{\partial T_{vs}}{\partial x_j} \simeq -\frac{\kappa_{vs}}{c_{v\,\mathrm{vibs}}}\frac{\partial e_{vs}}{\partial x_j}, \\ q_e &= -\kappa_e\frac{\partial T_e}{\partial x_j} \simeq -\frac{\kappa_e}{c_{ve}}\frac{\partial e_e}{\partial x_j}. \end{aligned} \tag{D.1}$$

This simplification is not mandatory, but it eases the derivation of M_η and the Jacobian N. In the matrix $M_{\eta\, i,1\frac{1}{2}}$, we have defined the quantities t_u and t_T depending on the boundary conditions being simulated.

$$\begin{aligned} t_u &= \begin{cases} 0, & \text{slip condition;} \\ 2, & \text{no-slip condition,} \end{cases} \\ t_T &= \begin{cases} 0, & \text{adiabatic condition;} \\ 2, & \text{fixed-wall temperature condition.} \end{cases} \end{aligned} \tag{D.2}$$

The Jacobian $N = \frac{\partial \mathbf{V}}{\partial U}$, which was defined for use in equation (3.3.20) is given below. The derivatives that appear in this expression are as follows.

$$
\begin{aligned}
\frac{\partial c_s}{\partial \rho_s} &= \frac{1}{\rho}\big(1 - c_s\big) \\
\frac{\partial c_s}{\partial \rho_r} &= -\frac{c_s}{\rho} \quad \text{for } s \neq r \\
\frac{\partial T}{\partial \rho_s} &= -c_{vs}T + \frac{1}{\rho c_v}\Big(\big(\frac{1}{2} - c_e\big)\big(u^2 + v^2\big) - h_s^\circ - e_{\mathrm{els}}\Big) \quad \text{for } s \neq e \\
\frac{\partial T}{\partial \rho_e} &= \frac{c_e}{\rho c_v}\big(u^2 + v^2\big) \\
\frac{\partial T}{\partial \rho u} &= \frac{u}{\rho c_v}\big(1 - c_e\big) \\
\frac{\partial T}{\partial \rho v} &= \frac{v}{\rho c_v}\big(1 - c_e\big).
\end{aligned}
\tag{D.3}
$$